

# CURRICULUM VITAE OF STEVE SCHEINER

## I. Personal

### Date and Place of Birth

February 27, 1951, New York, New York

### Present University Department

Department of Chemistry and Biochemistry  
(435) 797-7419

email: [scheiner@cc.usu.edu](mailto:scheiner@cc.usu.edu)

### Present Home Address

4770 Hollow Road, Logan, UT 84321  
(435) 245-0710

## II. Education

B.S. (Chemistry) City College of New York

May, 1972

A.M. (Chemistry) Harvard University

May, 1974

Ph.D. (Chemical Physics) Harvard University

November, 1976

## III. Professional Experience

Weizmann Postdoctoral Fellow: September, 1976 - August, 1978  
The Ohio State University, Columbus, Ohio 43210

Assistant Professor of Chemistry & Biochemistry: 1978 - 1982  
Southern Illinois University, Carbondale, Illinois 62901

Associate Professor of Chemistry & Biochemistry: 1982 - 1986  
Southern Illinois University, Carbondale, Illinois 62901

Professor of Chemistry & Biochemistry: 1986 - 2000  
Southern Illinois University, Carbondale, Illinois 62901

Professor of Chemistry & Biochemistry: 2000 - present  
Utah State University, Logan, Utah, 84322

## IV. Teaching Experience

### Teaching Interests and Specialties

Physical Chemistry, Molecular Orbital Theory, Group Theory, Spectroscopy,  
Quantum Chemistry, General Chemistry, Chemistry for Nonscientists

Student Completing Theses and Dissertations:

Neena L. Summers, PhD, July, 1984

A Quantum Mechanically Based Energy Partitioning Method (QMEP) for Polypeptide Conformation Prediction

Larry D. Bigham, MA, March, 1985

An ab initio Study of Proton Transfers in  $(S_2H_5)^+$  with Comparisons to  $(O_2H_5)^+$

Robert J. Brenstein, PhD, February, 1986

Theoretical Investigation of Compounds Containing Silicon-Oxygen Bonds

Eric A. Hillenbrand, PhD, April, 1986

A Study of Proton Transfers involving Hydroxyl, Amine, Imine, Carbonyl, and Carboxyl Groups

Paul C. Redfern, PhD, February, 1987

Theoretical Studies of Proton Transfer Reactions: Effects of External Ions, Test of Marcus Theory, and Hydrogen Exchange in Proteins

Ingrid J. Kurnig, PhD, April, 1988

Proton Transfer Potentials and Vibrational Spectra of H-Bonded Systems

Slawomir M. Cybulski, PhD, May, 1989

Ab Initio Studies of Hydrogen Bonding and Proton Transfers involving Simple and Multiply Bonded Systems

Wa-On Yu, MS, August, 1990

Effect of Proton Transfer on the Stability of an Adjacent Hydrogen Bond

Lan Wang, PhD, July, 1992

Energetics and Kinetics of Proton Transfer between Doubly-Bonded Atoms, Amides, and Anions

Xiaofeng Duan, PhD, May, 1993

Theoretical Studies of Proton Transfer along Inter- and Intramolecular Hydrogen Bonds

Martin Cuma, PhD, June, 1998

Theoretical Study of Isotope Effects in Hydrogen Bonding, Excited State Intramolecular Proton Transfer and Stability of Small  $BC_2N$  Clusters

Yanliang Gu, MS, July, 1999

Fundamental Properties of the  $CH\cdots O$  Interaction: Is It a True Hydrogen Bond?

Postdoctoral Fellows, Research Associates, and Visiting Faculty

M. M. Szczesniak, University of Wroclaw, Poland (1981-1991)

Z. Latajka, University of Wroclaw, Poland (1982-1986)

R. Brenstein, Southern Illinois University (1986-1988)

M. Remko (International Fulbright Scholar), University of Bratislava, Czechoslovakia (1987)  
M. Bulski, University of Warsaw (1987-1988)  
Z. Latajka, University of Wroclaw, Poland (1988)  
R. Wang, Northeast Normal University, China (1988)  
G. Chalasinski, University of Warsaw (1988-1989)  
Z. Latajka, University of Wroclaw, Poland (1989-90)  
V. Marudarajan, University of Southern California, (1989-1991)  
G. Chalasinski, University of Warsaw (1990)  
S. Cybulski, Ottawa University (1990-91)  
K. Luth, Ohio State University (1991-1994)  
G. Chalasinski, University of Warsaw (1991, 1992, 1993)  
Z. Latajka, University of Wroclaw, Poland (1991, 1992)  
J. Florian, Charles University, Prague, Czechoslovakia (1992- 1994)  
R. Wang, Northeast Normal University, China (1992)  
T. Kar, Indian Institute of Technology, India (1993- )  
M. Vener, Moscow University, Russia (1993-4)  
C. Rovira, University of Barcelona, Spain (1994)  
C. Thomson, Northwest Missouri State University (1994)  
J. Badenhoop, University of Wisconsin (1994-96)  
M. Yi, University of Singapore (1994-96)  
G. Orlova, University of Rostov, Russia (1996-7)  
M. Forés, University of Girona, Spain (1998)  
A. Isaev, Institute of Organic Chemistry, Moscow, Russia (1999)  
M. Liao, University of Puerto Rico (2000-2004 )  
S. Galembeck, Sao Paulo University (2002)

#### Undergraduate Students Supervised

Carl Leidhold, University of Massachusetts  
Sharon Yee, University of Maryland, Baltimore County  
Frederick Sahlen, University of Stockholm  
Kyle Burrell, SIUC  
Pam Stumphy, SIUC  
Andrew Phillips, SIUC  
Jim Spivey, SIUC  
Patrick Wheeler, Northeast Missouri State University  
Don Elmore, Grinnell College  
Justin Ego, USU

#### High School Students Supervised

Devon Brooks, Carbondale High School  
Tina Walker, Herrin High School  
Jacob Layton, Clearfield High School (2001)

Member of Graduate Committee for:

Aleksey Kuznetsov, Anastassia Alexandrova, Yu Hui, Aleksandra Mikosz, Ben Elliott, Magdalena M. Makowska-Grzyska, Amy Fuller, Gajendra Ingle, Dmitri Zoubarev, Boris Averkiev

## **V. University Service**

### Department Committees

Physical Chemistry Course Review Committee (1978-1979)  
Chemistry Conference Committee (1979-1982))  
Graduate Admissions Committee (1979-1984)  
Consortium Committee (1979-1980)  
Chairman, Seminar Committee (1984-1990)  
Chairman, Graduate Admissions Committee (1990-1993, 1995-present)  
Seminar Committee (1990-1992)  
Search Committee for Department Chair (1990)  
Department Chairman (1992-95)  
Faculty Search Committee (1998-99)  
Renovation Committee (1993-98)  
Tenure & Promotion Committee (1992-2000)  
Instructional Evaluation and Improvement Committee (1998-99)  
Faculty Search Committee (1999-2000)

### College and University Committees

Phi Beta Kappa Committee (1979-1981)  
Illinois Junior Science and Humanities Symposium Committee (1981-1984)  
University Academic Computing Advisory Committee (1984-1987)  
Search Committee, Associate Director of System Software, Computing Affairs (1985)  
College of Science "2% Return" Committee (1986-1987)  
Graduate Council (1986-1989)  
Research Committee - Graduate Council (1986-1989)  
Program Review Committee - Computer Science (1986-1987)  
Chair, Search Committee - Director of Office of Research Development & Administration and Associate Dean of Graduate School (1987-1988)  
College of Science Outstanding Researcher Selection Committee (1988-1990)  
University Outstanding Scholar Selection Committee (1988-1989)  
University Research Committee (1986-1989)  
University Planning Committee for New Science Building (1989-1990)  
University Outstanding Scholar Selection Committee (1993-96)  
Graduate Council (1995-1998)  
Member of University Grievance Panel (1996)  
Member of University Grievance Panel (1997)  
Member, Research Committee of Graduate Council (1995-1998)  
Chair, Search Committee for University Chancellor (1997-8)  
College of Science Personnel Committee (1998 - 2000)  
Member, Research Advisory Group to Chancellor's Planning & Budget Council (1999-2000)

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Chair, Search Committee - Director of Office of Research Development & Administration  
and Associate Dean of Graduate School 1999

Consortium for Advanced Radiation Sources (CARS) Advisory Board (1999 - 2000)

## **VI. Professional Service**

### Membership in Professional Associations

American Chemical Society  
American Physical Society  
International Society of Quantum Biology

### Offices Held and Honors Awarded in Professional Associations

Secretary, Local ACS Section, 1986  
Secretary-Treasurer, International Society of Quantum Biology, 1988-1992  
Executive Committee, International Society of Quantum Biology, 1993-96  
Appointed to Advisory Board, International Workshop on the Hydrogen Bond, (1999- )

### Consultantships

Served on Special NIH Study Section, July, 1983  
Served on Special NIH Study Section, June, 1984  
Served on Special NIH Study Section, December, 1984  
Outside Reviewer of Proposal for NIH, September, 1985  
Ad Hoc Member of NIH Study Section (BBCA), October, 1987  
Served on Special NIH Study Section, April, 1988  
Ad Hoc Member of NIH Study Section (BBCA), June, 1988  
Served on Special NIH Study Section, August, 1988  
Member of NSF Advisory Panel for the Biophysics Program, 1988-1989  
Outside reviewer for Habilitation degree application of M. Ramek, University of Graz, Austria, April, 1990  
Served on Special NIH Study Section, July, 1990  
Served on Special NIH Study Section, November, 1990  
Served on Special NIDA Study Section, August, 1991  
External Examiner for doctoral thesis of G.A. Yeo, University of Witwatersrand, South Africa, August, 1991  
Served on Special NIH Study Section, October, 1991  
Ad Hoc Member of NIH Study Section (BBCA), November, 1991  
Member, National Institutes of Health Reviewers Reserve, 1991-95  
Member of NIH Study Section (Shared Instrumentation Grants), October, 1993  
Member, Board of Examiners for doctoral thesis of P. K. Nandi, Indian Institute of Technology, Kharagpur, India, 1994.  
Asked to Evaluate Tenure Credentials of Faculty Member of the University of Missouri, Kansas City, 1994  
Ad Hoc Member of NIH Study Section (BBCA), June, 1998  
Asked to Evaluate Tenure Credentials of Faculty Member of St. Louis University, 1998  
Asked to Evaluate Promotion Dossier of Faculty Member of University of Natal, South Africa, 1998  
Member, Board of Examiners for doctoral thesis of S. B. Manna, Jadavpur University, Calcutta, India, 2001.  
Member, Board that makes annual ACS Utah Award (2004 - )  
Evaluator, Credentials of Professor, Universiteit Antwerpen, 2005  
Evaluator, Credentials of Professor, University of the West Indies, 2005



Evaluation of Manuscripts for Journals and Book Publishers and of Grant Proposals for Agencies  
(approximately 50 reviews of journal articles each year)

Journals

Science	J. Amer. Chem. Soc.
J. Chemical Physics	J. Physical Chemistry
Accounts of Chemical Research	Chem. Phys.
Chem. Phys. Letters	Biochemistry
Proc. Nat. Acad. Sci., USA	Radiochimica Acta
Macromolecules	J. Computational Chemistry
J. Theoretical Biology	Z. Naturforsch.
Molecular Pharmacology	International J. Quantum Chem.
J. Molecular Structure	J. Molecular Structure (Theochem)
Biopolymers	Structural Chemistry
Archives of Biochem. Biophys.	Canadian Journal of Chemistry
Journal of Crystal Growth	J. Organic Chemistry
Theoretica Chimica Acta	Chemical Reviews
J. Biological Chemistry	Computers & Chemistry
J. Pharmaceutical Sciences	Biophysical Chem.
Biochim. Biophys. Acta	Croat. Chem. Acta
New Journal of Chemistry	J. Physical Organic Chemistry
Biophysical Journal	Comput. Sci. Eng.
Photochemistry & Photobiology	Biospectroscopy
J. Molecular Liquids	Computers & Chemistry
Iranian Journal of Science & Technology	J. Biological Physics
J. Molecular Biology	Israel J. Chemistry
Organic Letters	Theoretical Chem. Accounts
Journal of Molecular Graphics & Modelling	Angewandte Chemie
Nature	Solid State Ionics
Proteins, Structure, Function and Genetics	ChemPhysChem
J. Photochem. Photobiol.	Inorganic Chemistry
J. Chemical Information & Computer Sciences	Molecular Physics
J Biomolecular and Structural Dynamics	Chemical Biology
Spectroscopy Letters	Radiation Physics and Chemistry
Physical Chemistry Chemical Physics	Proteins: Structure, Function, and Bioinformatics
Journal, Amer. Soc. for Mass Spectrometry	Organometallics
Journal of Chemical Information and Modeling	

Books

Oxford University Press  
Wiley Interscience  
American Chemical Society Books

Proposals

National Institutes of Health  
National Institutes of Health, Fellowship Program  
National Science Foundation, Chemistry Division



National Science Foundation, Biophysics Division  
National Science Foundation, International Programs  
National Research Council of Canada  
Petroleum Research Fund (American Chemical Society)  
City University of New York  
U. S.- Israel Binational Science Foundation  
Cornell Theory Center  
New York Academy of Sciences  
International Science Foundation  
National Research Council - COBASE program  
Civilian Research & Development Foundation  
South African National Research Foundation  
Austrian Science Fund, 2005

Papers Presented at Professional Meetings

Third East Coast Protein Crystallography Workshop, Lenox, MA, October, 1975.  
Second International Congress of Quantum Chemistry, New Orleans, LA, April, 1976.  
Ohio Theoretical Chemistry Conference, Cincinnati, OH, September, 1977.  
Eleventh Midwest Theoretical Chemistry Conference, Columbus, OH, May, 1978.  
American Conference on Theoretical Chemistry, Boulder, CO, June, 1978.  
American Chemical Society Great Lakes Region, Rockford College, Rockford, IL, June, 1979.  
NRCC/QCPE Workshop "Computational Methods for Molecular Structure Determination: Theory and Technique", Indiana University, Bloomington, IN, August, 1979.  
Sanibel Symposia: International Symposium on Quantum Biology and Quantum Pharmacology, Palm Coast, FL, March, 1980.  
Conference on Quantum Chemistry in Biomedical Sciences, New York, NY, June, 1980.  
Sanibel Symposia: International Symposium on Quantum Biology and Quantum Pharmacology, Palm Coast, FL, March, 1981.  
American Conference on Theoretical Chemistry, Boulder, CO, June, 1981.  
Fourth International Congress on Quantum Chemistry, Uppsala, Sweden, June, 1982.  
Quantum Chemistry in Biology, Stockholm, Sweden, June, 1982.  
Sixth International Symposium on the Physics and Chemistry of Ice, Rolla, MO, August, 1982.  
Second International Conference on Water and Ions in Biological Systems, Bucharest, Romania, September, 1982.  
Faraday Discussion No. 74: Electron and Proton Transfer, Southampton, England, September, 1982.  
Biophysical Society Meeting, San Diego, CA, February, 1983.  
Presented 5 papers at Midwest Theoretical Chemistry Conference, Evanston, IL, May, 1983.  
Organosilicon Symposium, Fargo, ND, June, 1983.  
Gordon Conference: Energy Coupling Mechanisms, Andover, NH, August, 1983.  
Invited Speaker to the US-Romanian Exchange Workshop on the Role of Water and Ions in Biological Membrane Function, Bandera, TX, February, 1984.  
Biophysical Society Meeting, San Antonio, TX, February, 1984.  
Sanibel Symposium on Quantum Biology and Quantum Pharmacology, Palm Coast, FL, March, 1984.  
Presented 3 papers at National Meeting, American Chemical Society, St. Louis, MO, April, 1984.  
Organosilicon Symposium, Schenectady, NY, April, 1984.

Presented 5 papers at 17th Midwest Theoretical Chemistry Conference, Carbondale, IL May, 1984.  
Invited Speaker at Conference on Molecular Basis of Cancer, Roswell Park Memorial Institute, Buffalo, NY, May, 1984.  
Presented 4 papers at the American Conference on Theoretical Chemistry, Jackson, WY, June, 1984.  
Invited Discussant to the 1984 Gordon Conference on the Biochemical Aspects of Photosynthesis, Meriden, NH, August, 1984.  
National Meeting of the American Chemical Society, Philadelphia, PA, August, 1984.  
Invited Speaker to the 1985 Gordon Conference on Protons and Membrane Reactions, Santa Barbara, CA, January, 1985.  
Presented 5 papers at Midwest Theoretical Chemistry Conference, Milwaukee, WI, May, 1985.  
Invited Speaker, Lipscomb Symposium, Denver, CO, June, 1985.  
Invited Speaker at Quantum Chemistry of Biological Systems, New York, NY, August, 1985.  
Presented 3 papers at International Congress of Quantum Chemistry, Montreal, Quebec, August, 1985.  
Presented 2 Invited Talks at "Horizons in H-Bond Research", Marburg, West Germany, September, 1985.  
Biophysical Society Meeting, San Francisco, CA, February, 1986  
Invited Plenary Speaker at Sanibel Symposia, Marineland, FL, March, 1986.  
Organosilicon Symposium, Tarrytown, NY, April, 1986.  
Presented 5 papers at Midwest Theoretical Chemistry Conference, Bloomington, IN, May, 1986.  
Gordon Conference on Computational Chemistry, New Hampshire, August, 1986.  
Symposium Leader and presented a paper at Sanibel Symposium, Marineland, FL, March, 1987.  
Eighth International Symposium on Organosilicon Chemistry, St. Louis, MO, June, 1987.  
Presented 3 papers at the American Conference on Theoretical Chemistry, Gull Lake, MN, July, 1987.  
Invited to deliver Plenary Lecture at the World Association of Theoretical Organic Chemists Congress in Budapest, Hungary, August, 1987 (unable to attend).  
Invited Plenary Speaker at International Workshop on the Hydrogen Bond, Polanica, Poland, September, 1987.  
Invited Speaker to the 1988 Gordon Conference on Protons and Membrane Reactions, Santa Barbara, CA, February, 1988.  
Sanibel Symposium, Marineland, FL, March, 1988  
Presented 3 papers at Midwest Theoretical Chemistry Conference, Argonne, IL, May, 1988  
Special Invited Lecture, International Symposium on the Electronic Structure and Properties of Molecules and Crystals, Dubrovnik, Yugoslavia, August, 1988  
Symposium on Quantum Chemistry, Tatranska Lomnica, Czechoslovakia, October, 1988.  
Sanibel Symposium, St. Augustine, FL March, 1989  
Presented 3 papers at Midwest Theoretical Chemistry Conference, Indianapolis, IN, May, 1989  
Invited Speaker, Symposium on Membrane Proteins as Transducers of Energy and Information, University of Virginia, Charlottesville, VA, May, 1989  
Invited Speaker at CECAM Workshop on Proton Transfer Reactions in Solution, Paris, France, July, 1989.  
Invited Speaker at ACS Symposium, Miami, FL, September, 1989  
Invited Speaker at International Hydrogen Bond Conference, Utrecht, Netherlands, September, 1989 (unable to attend)  
Sanibel Symposium, St. Augustine, FL, March, 1990

Invited Speaker at ACS Symposium, Boston, MA, April, 1990  
Invited Speaker to Lipscomb Symposium, Cambridge, MA, June, 1990  
Invited Speaker at Conference on Intermolecular Interactions in Chemistry and Biology: Theory and Experiment, Podebrady, Czechoslovakia, September, 1990  
Paper presented at Conference on Structure and Conformational Dynamics of Biomacromolecules, High Tatras, Czecho-Slovakia, September, 1990  
Invited Speaker to Conference on Photoinduced Proton Transfer Dynamics in Chemistry, Biology and Physics, Tallahassee, FL, January, 1991  
Talk presented at The Chemistry and Physics of Clusters and Cluster Ions, Baltimore, MD, January, 1991.  
Vice Chair of the 1991 Gordon Conference on Protons and Membrane Reactions, Ventura, CA, February, 1991.  
Sanibel Symposium, St. Augustine, FL, March, 1991.  
Invited Speaker at NATO Workshop on Proton Transfer in Hydrogen-Bonded Systems, Heraklion, Crete, Greece, May, 1991.  
two presentations at Sanibel Symposium, St. Augustine, FL, March, 1992.  
Paper presented at 5th Meeting in Bioorganic Chemistry, Liblice Castle, Czecho-Slovakia, April, 1992.  
presented 4 talks at XXV Midwest Theoretical Chemistry Conference, East Lansing, MI, June, 1992.  
Invited Speaker at Xth International Workshop in Hydrogen-Bond Research, Kiev, Ukraine, September, 1992 [meeting cancelled].  
three presentations at Sanibel Symposium, St. Augustine, FL, March, 1993.  
Two presentations at XXVI Midwest Theoretical Chemistry Conference, Carbondale, IL, May, 1993.  
Invited speaker at Summer School on Isotope Effects, Karpacz, Poland, June, 1993.  
Congress of the International Society for Theoretical Chemical Physics, Girona, Spain, July, 1993  
Invited speaker at Computers in Chemistry Symposium on Modeling the Hydrogen Bond, ACS National Meeting, Chicago, IL August, 1993  
Invited to speak at the Symposium on Quantum Tunneling, ACS National Meeting, Chicago, IL August, 1993  
Current Trends in Computational Chemistry, Jackson State University, November, 1993.  
Chair of the 1994 Gordon Conference on Protons and Membrane Reactions, Ventura, CA, February, 1994.  
Three presentations at XXVII Midwest Theoretical Chemistry Conference, Columbia, MO, May, 1994.  
Invited Speaker at Current Trends in Computational Chemistry, Vicksburg, MS, November, 1994.  
Sanibel Symposium, St. Augustine, FL, February, 1995.  
Molecular Quantum Mechanics: Methods and Applications, Cambridge, England, September, 1995.  
American Conference on Theoretical Chemistry, Park City, UT, July, 1996.  
Invited Speaker at Structural and Mechanistic Organic Chemistry, Athens, GA, June, 1997.  
Invited Speaker at International Discussion Meeting on Hydrogen Transfer: Experiment and Theory, Berlin, Germany, September, 1997.  
First Meeting of Researchers on Tunable Optical Polymers, Rochester, NY, May, 1999  
Nanotube 99, Lansing, MI, July, 1999  
World Congress of Theoretically Oriented Chemists, London, England, August, 1999  
Discussion Group on Tunable Optical Polymers, Adelphi, MD, July, 1999

Invited Speaker at International Workshop on the Hydrogen Bond, Swieradow, Poland, September, 1999

Invited Speaker to Symposium on Proton Transport at National ACS Meeting, August, 2000

Presentation of research results at Annual Meeting in Tunable Optical Polymers, Natick, MA, August, 2000

Invited Speaker to 8th European Symposium on Organic Reactivity (ESOR VIII), Cavtat/Dubrovnik, Croatia, September, 2001 (invitation declined)

Session Chair and Invited Speaker, Horizons in Hydrogen Bond Research, Torino, Italy, September 2001

Two presentations of research results at Annual Meeting in Tunable Optical Polymers, Cambridge, MA, March, 2002

Invited Speaker to Symposium on Chromogenic Phenomena in Polymers: Tunable Optical Properties at National ACS Meeting, Orlando, FL, April, 2002

International Conference on the Science and Application of Nanotubes, Boston, July, 2002

### Invited Seminar Speaker

Southern Illinois University, Edwardsville, October, 1978

Indiana University-Purdue University at Indianapolis, November, 1979

Merck, Sharp, and Dohme Research Laboratory, Rahway, NJ, January, 1981

Argonne National Laboratory, Argonne, IL, August, 1981

Indiana State University, Evansville, IN, October, 1981

Hunter College of City University of New York, NY, June, 1982

Villanova University, October, 1983

Abbott Laboratories, March, 1984

Eastern Illinois University, February, 1985

Emory University, March, 1985

University of Alabama, Birmingham, February, 1987

Florida State University, January, 1988

University of California, Los Angeles, February, 1988

University of Mississippi, March, 1988

University of Illinois, Urbana, September, 1988

University of New Mexico, October, 1988

Kansas University, December, 1988

Miami University, March, 1989

Comenius University, Bratislava, Czechoslovakia, September, 1990

University of Colorado, October, 1990

Carnegie-Mellon University, January, 1992

University of Missouri, St. Louis, February, 1993

Illinois State University, March, 1993

Beckman Institute, Urbana, IL, April, 1994

Indiana University-Purdue University at Indianapolis, September, 1994

Texas Tech University, March, 1995

University of Missouri, St. Louis, December, 1996

University of Toledo, March, 1997

Max-Planck-Institut for Festkörperforschung, Stuttgart, Germany, September, 1997

St. Louis University, October, 1997

University of Arizona, April, 1998  
Murray State University, October, 1999  
Utah State University, February, 2000  
Brigham Young University, March, 2002  
University of New Hampshire, October, 2002  
University of Maryland, Baltimore County, April, 2004

#### EDITORIAL BOARDS

Journal of Molecular Structure, Theochem (1991- 2007)  
Computational and Structural Chemistry (1999-2004)  
International Journal of Quantum Chemistry (2006-2010)

#### OTHER

Organized 17th Annual Midwest Theoretical Chemistry Conference, Carbondale, IL, May, 1984.  
Organized 26th Annual Midwest Theoretical Chemistry Conference, Carbondale, IL, May, 1993.  
Member of Scientific Committee: International Conference on Solid State Protonic Conductors, Stuttgart, Germany, August, 1994  
Edited a Special Issue of the Journal of Molecular Structure on Molecular Interactions  
Taught a course in the Winter School in Theoretical Chemistry, University of Helsinki, Finland, December, 1999  
General Chair, Program Co-Chair, and Treasurer for ACS Joint Northwest/Rocky Mountain Regional Meeting, June, 2004

### VII. Community Service

Judge at 1980, 1981, 1987. 1998 Science Fairs  
Judge at 1984 High School Chemistry Bowl

### VIII. Research

#### Research Interests and Specialties

Quantum Chemistry, Proton Transfers, Hydrogen Bonding

#### Current Research Projects

Proton Transfers, Theoretical Studies of Hydrogen Bonding, Excited State Proton Transfer, Unconventional Hydrogen Bonds, Tunable Optical Polymer Systems

#### Research Grants Applied for:

Research Corporation (1978)  
Petroleum Research Fund (1978)  
Petroleum Research Fund (1980)  
National Institutes of Health (1980)  
Southern Illinois University Research Projects (1980)  
National Science Foundation (1981)  
Dreyfus Teacher-Scholar Grant (1981)  
Sloan Research Fellowship (1981)  
NIH Research Career Development Award (1981)  
Southern Illinois University Research Projects (1982)

NSF Chemical Instrumentation Program (1983)  
NSF Presidential Young Investigator Award (1983)  
Department of Defense-University Research Instrumentation Program (1983)  
National Institutes of Health (1983)  
NSF Chemical Instrumentation Program (1983)  
National Institutes of Health Supplement (1984)  
National Science Foundation (1984)  
Harris Corporation (1984)  
National Science Foundation (1985)  
National Institutes of Health (1985)  
National Science Foundation (1986) [Supercomputer Usage Proposal]  
National Science Foundation (1986)  
National Institutes of Health (1986)  
San Diego Supercomputer Center (1987)  
National Center for Supercomputing Applications (1987)  
San Diego Supercomputer Center (1988)  
San Diego Supercomputer Center (1988)  
National Center for Supercomputing Applications (1988)  
National Institutes of Health (1988)  
IBM (1989)  
National Center for Supercomputing Applications (1989)  
National Institutes of Health (1989)  
National Science Foundation (1989)  
National Institutes of Health (1990)  
National Science Foundation (1991)  
National Science Foundation, US-Eastern Europe Cooperative Science Program (1992)  
National Science Foundation, Conference Support Grant (1993)  
National Institutes of Health, Conference Support Grant (1993)  
National Science Foundation, Academic Research Infrastructure (1993)  
National Research Council, CAST program (1993)  
International Science Foundation Travel Grant Program (1993)  
National Institutes of Health (1993)  
National Institutes of Health (1994)  
U.S. Department of Education, Graduate Assistance in Areas of National Need (1994)  
NSF, REU Program (1995)  
National Research Council, CAST program (1996)  
CRDF, (1996)  
National Science Foundation (1996)  
U.S. Department of Education, Graduate Assistance in Areas of National Need (1996)  
National Institutes of Health (1997)  
Southern Illinois University Research Projects (1997)  
Southern Illinois University Summer Research Fellowship (1997)  
National Science Foundation (1997)  
Petroleum Research Fund - American Chemical Society (1997)  
National Research Council, COBASE program (1998)  
Multidisciplinary University Research Initiative, Office of Naval Research (1998)

U.S. Department of Education, Graduate Assistance in Areas of National Need (1999)  
Civilian Research and Development Foundation (1999)  
National Science Foundation (2000)  
Space Power Technology Division of NASA (2000)  
National Science Foundation (2002) [PI: Kar, Co-PI: Scheiner]  
Beckman Foundation Scholars Program (2002)  
National Institutes of Health (2002)  
Binational Science Foundation (2002) Proton transfer reactions in the solute-solvent interaction domain, \$50,000 (Co-PI with M. Gutman)  
National Science Foundation (2002) Porphyrin-Metal Interactions, \$519,570  
National Institutes of Health (2003) Determination of hydrogen-bond energy in biomolecules, \$1,100,000  
National Institutes of Health (2003) CH--O Hydrogen Bonds,

**D. Research Grants Received: (\$3.7 M in external funds)**

Research Corporation (\$5,400), March, 1979  
Southern Illinois University Research Projects, 1980-82  
National Institutes of Health, General Medical Sciences (\$156,000 direct costs), 1981-84  
NIH Research Career Development Award (\$173,000), 1982-87  
Southern Illinois University Research Projects, 1982-84  
National Institutes of Health, General Medical Sciences (\$423,000 direct costs), 1984-89  
Harris Corporation (\$64,640 direct costs), September, 1984  
National Institutes of Health Supplement, 1985 (award declined)  
National Science Foundation (1986) [Supercomputer Allocation: 25 hours]  
National Science Foundation (1987) [Supercomputer Allocation: 50 hours]  
National Institutes of Health, General Medical Sciences (\$230,500 direct costs), 1987-90  
San Diego Supercomputer Center (1987) [Supercomputer Allocation: 30 hours]  
National Center for Supercomputer Applications (1988) [Allocation: 48 hours]  
San Diego Supercomputer Center (1988) [Allocation: 180 hours]  
National Center for Supercomputer Applications (1988) [Allocation: 100 hours]  
National Institutes of Health, General Medical Sciences (\$529,000 direct costs), 1989-94  
IBM, 300 CPU hours on 3090-200VF, September, 1989  
National Institutes of Health, General Medical Sciences (\$486,000 direct costs), 1990-95  
National Science Foundation (1990) [award declined]  
National Science Foundation (\$121,000 total costs), 1992 - 1995  
National Research Council, CAST program (\$11,100) 1993-4  
National Science Foundation, Conference Support Grant (1993), \$3,000  
National Institutes of Health, Conference Support Grant (1993), \$5,000  
International Science Foundation Travel Grant Program (1993), \$900  
National Science Foundation, Academic Research Infrastructure (1993) \$734,000  
National Research Council, CAST program (1996), \$21,000  
Southern Illinois University Summer Research Fellowship (1997), one month summer salary  
National Institutes of Health, General Medical Sciences (\$488,000 direct costs), 1998-2002  
National Research Council, COBASE program (\$13,000 direct costs), 1999-2000

Multidisciplinary University Research Initiative, Army Research Office (\$238,000 direct costs)  
1999-2004

Binational Science Foundation, Proton transfer reactions in the solute-solvent interaction domain,  
\$50,000 (Co-PI with M. Gutman) 2003-2007

IUPAC, Categorizing hydrogen bonding and other intermolecular interactions (\$14,000 direct costs)  
2004-06

#### A. Invited Chapters in Professional Books

1. S. Scheiner  
"Molecular Orbital Treatment of Hydrogen Bonded Systems" in "Aggregation Processes in Solution", Stud. Phys. Theor. Chem., 26, Eds. E. Wyn-Jones, J. Gormally, Elsevier Scientific Publishing Co., Amsterdam, 1983, pp. 462-508.
2. S. Scheiner  
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