RALPH A. WHEELER
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EDUCATION and TRAINING

University of Houston: Postdoctoral Research Fellow, Computational Biophysics
Cornell University: PhD, Applied Computational Chemistry
Harvey Mudd College: BS, Chemistry

EMPLOYMENT

Northern Illinois University Department of Chemistry and Biochemistry

- Professor 2016-
- Department Chair 2016-2023

Duquesne University: Professor and Chair, Chemistry and Biochemistry 2010-2016

University of Oklahoma Department of Chemistry & Biochemistry:

- Presidential Professor 2003-2010
- Professor 1999-2010
- Associate Professor 1996-1999
- Assistant Professor 1990-1996
- Director, Supercomputing Lab for Electronic Properties of Materials 1996-2003

Scripps Research Institute: Visiting Professor, Molecular Biology 2006
UC-San Francisco: Visiting Associate Professor, Pharmaceutical Chemistry 1997-1998
Univ of Stockholm: Visiting Grad Assistant, Inst for Theoretical Physics Sep-Dec 1986

HONORS, AWARDS, and LECTURESHIPS

Fellow of the American Chemical Society	2010
Famous Overseas Professor Lectureship, Guangdong Province, PRC	2017
American Chem Soc Computers in Chem Division Outstanding Service Awards	2009, 2004
President's Associates Presidential Professor, University of Oklahoma	2003-2010
Regents' Award for Superior Research, University of Oklahoma	2002
Junior Faculty Research Fellowships, University of Oklahoma	1993, 1991, 1990
National Institutes of Health National Research Service Award	1989
National Research Council Postdoctoral Fellowship (declined)	1987
Cornell University Chemistry Dept., special teaching commendation	1983
American Chemical Society undergraduate research award	1982
Sigma Xi Honorary Research Society	1982
ARCS Foundation Scholarship	1981-1982
National Merit Scholarship	1978-1982
National Society of Professional Engineers Scholarship	1978-1980

PRIMARY RESEARCH ACCOMPLISHMENTS

(1) Adapted signal/image processing methods to computational chemistry:

- Introduced modeling of small angle X-ray (SAXS) and neutron scattering (SANS) lineshapes to calculate distances and estimate aggregate sizes from experimental data.

- Used lineshape modeling to provide the first experimentally-based estimates of the nanoscale size of polar aggregates in ionic liquids.
- Wrote and distributed *viewSq*, a module for Visual Molecular Dynamics (VMD) capable of calculating X-ray or neutron total or partial structure factors, as well as quantifying and visualizing atomic contributions at chosen wavenumbers.
- First to use principal component analysis to calculate vibrational frequencies *and modes* for small molecules in the condensed phase.

(2) Implemented Extended Broken Symmetry approximation with *Gaussian09/Gaussian16* for using spin projection methods to calculate geometries and vibrational frequencies of spin-coupled transition metal clusters.
(3) Tested accuracy of density functional quantum chemistry for characterizing quinoidal and amino acid side chain radicals important in biological electron transfer.

TEACHING ACCOMPLISHMENTS

- Twice nominated by undergraduates for university-wide teaching awards (1990, 2013).
- Taught 17 different lecture courses at the University of Oklahoma, Duquesne University, and Northern Illinois University in General, Physical, and Inorganic Chemistry at graduate and undergraduate levels.

STUDENTS MENTORED

- Md Jasim Uddin Sohel (co-advised PhD student, 11/23-present)
- Timothy Huber (PhD candidate, 1/19-present)
- Emily Dalby (PhD 8/23)
- Mark Taylor (MS 10/22; Teacher at Walter Payton College Preparatory High School)
- Ashlyn Koval (PhD 8/19; Postdoctoral, US Army Corps of Engineers)
- Travis Mackoy (PhD 5/19; Associate Data Scientist, Prognos Healthcare Analytics)
- Baolinh Nguyen (PhD 4/13; Postdoctoral, University of Texas Medical Branch)
- Zhanyong Guo (Ph.D. 7/08; Postdoctoral, University of Texas-Arlington)
- Tim Click (Ph.D. 8/07; NIH Predoctoral Fellow; Postdoctoral, Central Michigan University)
- C. Adam Hixson (Ph.D.12/06; University of Oklahoma Alumni Fellow; Departmental Research Excellence Award; Postdoctoral, University of Pittsburgh)
- Zun-nan “Victor” Huang (Ph.D. 11/05; Outstanding Overseas Chinese Student Scholarship; Postdoctoral, Univ. of Missouri-St. Louis)
- Haitao Dong (Ph.D. 12/03; Postdoctoral, University of Delaware)
- Kris E. Wise (Ph.D. 4/99; National Research Council Postdoctoral Fellow, NASA)
- Anthony Kurt Grafton (Ph.D. 6/98; Assistant Professor, Campbellsville University, KY; OU Graduate College Research Award, Departmental Teaching and Research Excellence Awards)
- Han Zheng (M.S. thesis, 7/04; graduate student, New York University)
- Jermont Chen (M.S. thesis, 2/03; Lecturer, U.S. Air Force Academy; Colorado Springs, CO)
- Christian Matthaüs (M.S. thesis, 4/00; graduate student, City University of New York)
- Kevin S. Raymond (M.S. 11/97; high school science teacher)
- Scott E. Boesch (M.S. thesis, 9/96; Departmental Graduate Research Excellence Award).
- 30 undergraduates have conducted research in my group and have co-authored five publications.

NATIONAL/INTERNATIONAL STUDENT AWARDS to researchers in my group

- Goldwater Scholarships, 2014 (Ben Jagger); 2007 (Kurt Brorsen); 2006 (Sara Francis).
- American Chemical Society Computers in Chemistry Division CCG Excellence Awards to graduate students: 2006 (Tim Click); 2005 (Zun-Nan Huang); 2004 (C. Adam Hixson); 2003 (Haitao Dong)
- Outstanding Overseas Chinese Student Scholarship, 2003 (Zun-Nan Huang, graduate student).
- National Institutes of Health Predoctoral Fellowship for Students with Disabilities, 2003-2006 (Tim Click).
- Fulbright Fellowship, 2002 (Emily Reigh, undergraduate).
- National Science Foundation Predoctoral Fellowship, 2000 (Christine (Tratz) Aikens, undergraduate).
- National Science Foundation Professional Opportunities for Women in Research and Education (POWRE) award (Dr. Angela K. Wilson, postdoctoral researcher, one of only 6 chemists nationwide to win the NSF/POWRE award in 1999).
- National Research Council Postdoctoral Fellowship, 1999 (Kris Wise, graduate student).

NATIONAL/INTERNATIONAL SERVICE

- Member, American Chemical Society Committee on Science, 1/09-12/2020.
- Councilor, American Chemical Society Computers in Chemistry Division, 1/09-12/17.
- Governing Board Member, Council for Chemical Research (CCR), 1/14-9/17.
- Editorial Board Member, Journal of Molecular Graphics and Modeling (publication of the Molecular Graphics Society and the ACS Computers in Chemistry Division), 6/98-2017.
- Editor, Annual Reports in Computational Chemistry, 10/08-12/14; Co-Editor, 3/06-10/08.
- Chair-Elect, Chair, Past Chair American Chemical Society Computers in Chemistry Division; 1/06-12/06, 1/07-12/07, 1/08-12/08, respectively.
- Editor, “Emerging Science” section, Annual Reports in Computational Chem., 6/03-3/06.
- Faculty representative to Federal Demonstration Partnership to streamline grant application and reporting requirements, 2002-2010.
- Alternate Councilor, American Chem Soc Computers in Chemistry Division; 9/03-12/06.
- Program Chair, American Chemical Society Computers in Chemistry Division; 3/00-3/04.
- Vice Program Chair, American Chem. Soc. Computers in Chemistry Division; 4/97-3/00.
- Invited participant in National Academy of Sciences workshop “Challenges for the Chemical Sciences in the 21st Century: Information & Communications” to consider national research priorities in computational chemistry, 10/31/02-11/2/02.
- Organized “Bioenergetics” symposium at 218th ACS National Meeting, August 1999.
- Reviewer: NSF, NIH, National Research Council, ACS/PRF, Research Corp., Biotechnology and Biological Sciences Research Council of the UK; many journals.

CURRENT GRANT SUPPORT

$341,653 / 4 NSF/Major Research Instrumentation; co-PI for “MRI: Acquisition of a 400 MHz NMR Spectrometer for Research and Education”; July 1, 2021- June 30, 2024.

$1,000,000/3 National Science Foundation/Scholarships for STEM Students (S-STEM); PI for “Scholarships and Enhanced Mentoring to Support Graduation of Students in Science and Mathematics”; January 15, 2019 to December 31, 2024.

PROPOSALS PENDING

$2,000,000/4 National Science Foundation/Scholarships for STEM Students (S-STEM); PI for "Scholarships for Equity and Excellence at Northern Illinois University"; January 2, 2025 to December 31, 2029; Submitted March 11, 2024.

EQUIPMENT GRANTS

$253,583 / 5 NSF/Major Research Instrumentation; co-PI for "MRI: Acquisition of Liquid Chromatograph/Mass Spectrometer for Research and Education"; July 1, 2017-June 30, 2020.

$254,796 / 5 National Science Foundation/Major Research Instrumentation; co-PI for "MRI: Acquisition of Large Shared Memory Supercomputer at Duquesne University"; August 1, 2011-July 31, 2014.

$792,925/17 National Science Foundation/Major Research Instrumentation Program; "MRI: Acquisition of Extensible Petascale Storage for Data Intensive Research"; October 1, 2010-September 30, 2014.

$250,000 / 21 National Science Foundation/CI-TEAM Program; "CI-TEAM: Cyberinrastructure for Bioinformatics and Beyond" December 1, 2006 to November 30, 2008.

$128,728 / 4 National Science Foundation;
"Acquisition of an Integrated Fourier Transform Raman/Microscope for Advanced Battery Materials Research and Student Training";
September 2001-August 31, 2002;
Funding for collaborators' vibrational spectroscopic equipment.

$100,000 / 6 National Science Foundation/Biological Instrumentation Program;
"An EPR Spectrometer for Protein and Metal Spin Resonance Analyses";
November 1996; Funding for 6 investigators to purchase EPR spectrometer.

$201,771 National Science Foundation/Silicon Graphics, Inc.;
"Graphics Supercomputer Laboratory"; December 1995; Funding for 4-processor Silicon Graphics Power Challenge graphics supercomputer.

$1,140,238/11 IBM Corporation/University of Oklahoma; "IBM SP2 Collaboration"; October 1995; Funding for 11 investigators to purchase 8-processor IBM SP2 supercomputer.

PAST GRANT SUPPORT

$80,000 / 2 Northern Illinois University/Diversity, Equity, and Inclusion (DEI) Postdoctoral Fellowship; "Chemistry—Discipline-based Education Research"; August 27, 2018-August 26, 2021.

$275,000 / 2 National Science Foundation/Research Experience for Undergraduates; PI for "REU site: Integrated computational and experimental REU site at Northern Illinois University"; March 1, 2017-February 29, 2020.

$617,680 / 5	National Science Foundation/Scholarships in Science, Technology, Engineering and Mathematics Program; “Scholarships for Academically Talented and Financially Disadvantaged Undergraduate and Graduate Students”; July 1, 2013 to June 30, 2018.
$135,000 direct costs	Oklahoma Center for Advancement of Science and Technology (OCAST). “Modeling electron transfer cofactors of cytochrome bc1”; June 1, 2007 to November 30, 2010.
827,800 cpu hours	National Science Foundation/National Resource Allocations Committee; 1994 to March 31, 2006.
$385,500	National Science Foundation/Theoretical and Computational Chemistry “Principle mode analysis and its application to polypeptide vibrations”; May 15, 2004 to May 14, 2007.
$80,296 direct costs	National Institutes of Health/Predoctoral Fellowships for Students with Disabilities; “Testing New Methods for Structure Prediction and Free Energy Calculations of Organics Molecules, Polypeptides, and Prion Proteins”; August 16, 2003-August 15, 2006 (Fellowship to Timothy Click).
$740,000	U.S. Department of Energy/Office of Science/Office of Basic Energy Science; "Quinone Binding and Reduction in the Photosynthetic Reaction Center"; September 1, 1997-May 31, 2004;
$135,000 direct costs	Oklahoma Center for Advancement of Science and Technology (OCAST); "New Method for Modeling Biomolecular Structures"; July 1, 2001 to June 30, 2004.
$523,000/18	National Science Foundation; "Center for Photonic and Electronic Materials and Devices"; February 1, 1998 to January 31, 2001; Center funding for 18 investigators.
$195,000 direct costs	Oklahoma Center for Advancement of Science and Technology (OCAST); "Quinone Binding and Reduction in Photosynthesis"; June 1, 1993 to May 31, 1996 and June 1, 1997 to May 31, 2000.
$100,000	National Science Foundation/Theoretical & Computational Chemistry; "Gas- and Solution-Phase Properties of Aromatic Amino Acid Radicals"; February 1, 1995 to May 31, 1997.
$30,000	National Institutes of Health; "Stabilities of Tyrosine and Tryptophan Radicals"; September 30, 1993 to September 29, 1994.
$18,000	American Chemical Society/Petroleum Research Fund; "Excess Electrons on Semiconductor Crystallites: Quantum Dynamical Studies";

September 1, 1990-August 31, 1992.

$44,765 University of Oklahoma Research Council;
Eight competitive research grants; June 1, 1990 to February 1, 1995.

$484,000/15 University of Oklahoma/Alumni Graduate Research Fellowships (3 separate grants); "Graduate Research Fellowships for the Department of Chemistry & Biochemistry"; August 15, 1998-August 31, 2006.

PUBLICATIONS (cited more than 3400 times, 44 citations per paper; h-index = 37)

83. Huber, T.; Wheeler, R.A.; “Fixed-node diffusion quantum Monte Carlo shows promise for modeling reaction thermochemistry of hydrocarbon-based radicals”; *J. Chem. Theory Comput.* **2024**; Submitted.

82. Vernier, B.; Patel, D.; Wheeler, R.A.; “Disordered nanocrystallite structural model for the ionic liquid 1,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide”; *Phys. Chem. Chem. Phys.* **2024**; Submitted.

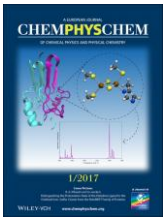
81. Wheeler, R.A.; Dalbey, Emily E.; “Structure factor lineshape model gives approximate nanoscale size of polar aggregates in the ionic liquid N-methyl-N-propylpyrrolidinium bis(trifluormethylsulfonyl)imide”; *Phys. Chem. Chem. Phys.* **2021**; *23*, 9061-9064.
Featured on the cover as one of the best papers in this issue

80. Mackoy, Travis; Kale, Bharat; Papka, Michael E.; Wheeler, R.A.; “viewSq, a Visual Molecular Dynamics (VMD) module for calculating, analyzing, and visualizing X-ray and neutron structure factors from atomistic simulations”; *Comput. Phys. Commun*. **2021**; *264*, 107881-/1-11. Corrigendum: *Comput. Phys. Commun.* **2022**; *276*, 108358-1/-11.

79. Mackoy, Travis; Mauro, Nicholas A.; Wheeler, R.A.; “Temperature dependence of static structure factor peak intensities for a pyrrolidinium-based ionic liquid”; *J. Phys. Chem. B* **2019**, *123*, 1672-1678.

78. Cooper, E.; Shaik, S.; Bautista, D.; Ahmed, A.; Gaetano, C.; Hockman, M.; Kochanek, S.; Jagger, B.R.; Richards, S.; Schmucker, C.; Roeske, L.; Renk, E.; Daley, K.; Romeo, J.; Wilding, M.; Biernesser, A.; Noonan, S.; Matosziuk, L.; Wheeler, R.A.; Vaidyanathan, N.; Johnson, P.; Gawalt, E.S.; Evanseck, J.D.; “Evolution of an AwSOME Chapter”; *ACS Symposium Series* **2018**, *1278* (“Building and maintaining award-winning ACS student member chapters”, Vol. 3); 55-71; American Chemical Society: Washington, DC.

77. Koval, Ashlyn M.; Jagger, Benjamin R.; Wheeler, R.A.; “Distinguishing the protonation state of the histidine ligand to the oxidized iron-sulfur cluster from the mitoNEET family of proteins“; *ChemPhysChem* **2017**, *18*, 39-41: http://dx.doi.org/10.1002/cphc.201600957.
Featured on the cover as one of the best papers in this issue.



76. Jagger, Benjamin R.; Koval, Ashlyn M.; Wheeler, R.A.; “Distinguishing protonation states of histidine ligands to the oxidized Rieske iron-sulfur cluster through ^{15}N vibrational frequency shifts”; *ChemPhysChem* **2016**, *17*, 216-220; http://dx.doi.org/10.1002/cphc.201500838.
Featured on the cover as one of the best papers in this issue.

75. Laury, Marie L.; Boesch, Scott E.; Haken, Ian; Sinha, Pankaj; Wheeler, R.A.; Wilson, Angela K.; “Harmonic vibrational frequencies: Scale factors for pure, hybrid, hybrid meta, and double-hybrid functionals in conjunction with correlation consistent basis sets”; *J. Comput. Chem.* **2011**, *32*, 2339-2347.

74. Giffin, Guinevere A.; Boesch, Scott E.; Bopege, Dharsani, N.; Powell, Douglas R.; Wheeler, R.A.; Frech, Roger; “Vibrational spectroscopy of secondary amine salts: 1. Assignment of NH_2^+ stretching frequencies in crystalline phases”; *J. Phys. Chem. B* **2009**,*113*, 15914-15920.

73. Boesch, Scott E.; Wheeler, R.A.; “Isotropic ^{13}C hyperfine coupling constants distinguish neutral from anionic ubiquinone-derived radicals”; *ChemPhysChem* **2009**, *10*, 3187-3189.

72. Hixson, C. Adam; Wheeler, R.A.; “Pressure annealing as a complement to temperature annealing to find low-energy structures of oligomeric molecules”; *J. Chem. Theory Comput.* **2009**, *5*, 1883-1894.

71. Bender, Shana L.; Keough, James, M.; Boesch, Scott E.; Wheeler, Ralph A.; Barry, Bridgette; “The vibrational spectrum of the secondary electron acceptor, A_1, in photosystem I”; *J. Phys. Chem B* **2008**; *112*; 3844-3852.

70. Huang, Zunnan; Wong, Chung; Wheeler, R.A.; “Flexible protein-flexible ligand docking with disrupted velocity simulated annealing”; *Proteins: Structure, function, bioinformatics* **2008**, *71*, 440-454.

69. Yoneda, Juliane D.; Albuquerque, M.G.; Leal, Katia Z.; Seidl, Peter R.; Wheeler, R.A.; Boesch, Scott E.; de Alencastro, R.B.; de Souza, M.C.B.V.; Ferreira, Vitor F.; “Molecular dynamics simulations of a nucleoside analogue of 1,4-dihydro-4-oxoquinoline-3-carboxylic acid synthesized as a potential antiviral agent: conformational studies in vacuum and in water”; *J. Molec. Struc. (Theochem)* **2006**, *778*, 97-103.

68. Carter, Shawn M.; Lee, Jonghyuk; Hixson, Christopher Adam; Powell, Douglas R.; Wheeler, R.A.; Shaw, Michael J.; Richter-Addo, George B.; “Fiber-optic infrared reflectance spectroelectrochemical studies osmium and ruthenium nitrosyl porphyrins containing alkoxide and thiolate ligands”; *J. Chem. Soc. Dalton Trans.* **2006**, 1338-1346.

67. Rahaman, Asif; Wheeler, R.A.; “Wavelet Transforms for Determining Time-Dependent Vibrational Frequencies”; *J. Chem. Theory Comput.* **2005**, *1*, 769-771.
One of the most frequently accessed papers from *J. Chem. Theory Comput.* during 3rd and 4th quarters of 2005: http://pubs.acs.org/journals/jctcce/promo/most_accessed/index.html

66. Dong, Haitao; Wheeler, R.A.; “Ultrafast Vibrational Energy Transfer from O-H Stretching Vibrations of Liquid Water”; *Chem. Phys. Lett.* **2005**, *413*, 176-181.

65. Sinha, Pankaj; Boesch, Scott E.; Gu, Changming; Wheeler, R.A.; Wilson, Angela K.; "Harmonic Vibrational Frequencies: Scaling Factors for HF, B3LYP, and MP2 Methods in Combination with Correlation-Consistent Basis Sets"; *J. Phys. Chem. A* **2004**, *108*, 9213-9217.

64. Wheeler, R.A.; "Simulating Thermochemistry of p-Benzoquinone Reduction in Water and Ubiquinone Binding in the Photosynthetic Reaction Center" in *Molecular Bioenergetics: Simulations of Electron, Proton, and Energy Transfer*; R.A. Wheeler, ed.; *ACS Symposium Series*: Washington, DC, **2004**, pp. 51-69.

63. Hixson, Christopher Adam; Chen, Jermont; Huang, Zunnan; Wheeler, R.A.; "New Perspectives on Multiple-Copy Mean-Field Molecular Dynamics Methods"; *J. Molec. Graphics and Modeling* **2004**, *22*, 349-357 (invited review).

62. Hixson, Christopher Adam; Wheeler, R.A.; "Practical Multiple-Copy Methods for Sampling Classical Statistical Mechanical Ensembles"; *Chem. Phys. Lett.* **2004**, *386*, 330-335.

61. Rahaman, Asif; Wheeler, R.A.; "Potential Energy Landscape for Conformationally Gated, Secondary Ubiquinone Binding in the Photosynthetic Reaction Center of Rhodobacter sphaeroides"; *ChemPhysChem* **2004**, *5*, 249-252.

60. York, Shawna; Boesch, Scott E.; Wheeler, R.A.; Frech, Roger; "Vibrational Assignments of High Molecular Weight Linear Polyethylenimine (LPEI) Based on Monomeric and Tetrameric Model Compounds"; *Macromolecules* **2003**, *36*, 7348-7351.

59. Wheeler, R.A.; Dong, Haitao; "Optimal Spectrum Estimation in Statistical Mechanics"; *ChemPhysChem* **2003**, *4*, 1227-1230.
Featured in *Chemical & Engineering News*, Feb. 9, 2004, pp. 30-31.

58. Wheeler, R.A.; Dong, Haitao; Boesch, Scott E.; "Quasiharmonic Vibrations of Water, Water Dimer, and Liquid Water from Principal Component Analysis of Quantum or QM/MM Trajectories"; *ChemPhysChem* **2003**, *4*, 382-384.
Featured in *Chemical & Engineering News*, Feb. 9, 2004, pp. 30-31.

57. Sanders, Rebecca A.; Boesch, Scott E.; Snow, Albert G.; Hu, Lieyu (Richard); Frech, Roger; Wheeler, R.A.; Glatzhofer, Daniel T.; "N,N,N',N',N"-Pentamethyldiethyltriamine (PMDETA) as a Model Compound for Linear Poly(N-Methylethylenimine), LPMEI"; *Polym. Preprints* **2003**, *44*, 966-967.

56. York, Shawna; Boesch, Scott E.; Wheeler, R.A.; Frech, Roger; "Effect of Lithium Triflate and Lithium Bromide on the Vibrational Frequencies of Dimethylethylenediamine (DMEDA)"; *J. Chem. Soc., Phys. Chem. Commun.* **2002**, *5*, 99-111 (electronic publication available at http://www.rsc.org/is/journals/current/ PhysChemComm/pcccon.htm).

55. Dong, Haitao; Hyun, Jin-Kee; Rhodes, Christopher P.; Frech, Roger; Wheeler, R.A.; "Molecular Dynamics Simulations and Vibrational Spectroscopic Studies of Local Structure in Tetraglyme:Sodium Triflate ($CH_3O(CH_2CH_2O)_4CH_3$:$NaCF_3SO_3$) Solutions"; *J. Phys. Chem. B* **2002**, *106*, 4878-4885.

54. Walden, Susan E.; Wheeler, R.A.; "Protein Conformational Gate Controlling Binding Site Preference and Migration of Ubiquinone-B in the Photosynthetic Reaction Center of *Rhodobacter sphaeroides*"; *J. Phys. Chem. B* **2002**, *106*, 3001-3006.

53. Hixson, Christopher Adam; Wheeler, R.A.; “Rigorous Classical-Mechanical Derivation of a Multiple Copy Algorithm for Sampling Statistical Mechanical Ensembles”; *Phys. Rev. E: Stat. Phys.* **2001**, *64*, 026701/1—026701/6.

52. Richter-Addo, George B.; Wheeler, R.A.; Hixson, Christopher Adam; Chen, Li; Khan, Masood A.; Ellison, Mary K.; Schulz, Charles E.; Scheidt, W. Robert; “Unexpected Nitrosyl Group Bending in Six-Coordinate $\{MNO\}^6$ σ-Bonded Aryl-(iron) and -(ruthenium) Porphyrins”; *J. Am. Chem. Soc.* **2001**, *123*, 6314-6326.

51. Dong, Haitao; Hyun, Jin-Kee; Durham, Curtis; Wheeler, R.A.; “Molecular Dynamics Simulations and Structural Comparisons of Amorphous Poly(ethylene oxide) and Poly(ethylenimine) Models”; *Polymer* **2001**, *42*, 7809-7817.

50. Hyun, Jin-Kee; Dong, Haitao; Rhodes, Christopher P.; Frech, Roger; Wheeler, R.A.; “Molecular Dynamics Simulations and Spectroscopic Studies of Amorphous Tetraglyme ($CH_3O(CH_2CH_2O)_4CH_3$) and Tetraglyme:$LiCF_3SO_3$”; *J. Phys. Chem. B* **2001**, *105*, 3329-3337.

49. Matthaüs, Christian; Wheeler, R.A.; “Fragment Mode Analysis and its Application to the Vibrational Normal Modes of Boron Trichloride-Ammonia and Boron Trichloride-Pyridine Complexes”; *Spectrochim. Acta A* **2001**, *57*, 523-536.

48. Wheeler, R.A.; “Quinones and quinoidal radicals in photosynthesis”; *Theoret. Comput. Chem.* **2001**, *9*, 655-690 (Invited review).

47. Boesch, Scott E.; York, Shawna; Frech, Roger; Wheeler, R. A.; “Experimental and Computational Investigation of the Structure and Vibrations of Dimethylethylenediamine, a Model for Poly(ethylenimine)”; *J. Chem. Soc., Phys. Chem. Commun.* **2001**, *4*, 1 (electronic publication).

46. Skokov, Sergei; Wheeler, R.A.; "Ab initio Molecular Dynamics Shows Low-Frequency Mode Manifolds Mediate $CO^+ + CO \rightarrow CO + CO^+$ Electron Exchange"; *J. Phys. Chem. A* **2000**, *104*, 6314-6323.

45. Razeghifard, M. Reza; Kim, Sunyoung; Patzlaff, Jason; Hutchison, Ronald, S.; Krick, Thomas; Ayala, Idelisa; Steenhuis, Jacqueline J.; Boesch, Scott E.; Wheeler, R. A.; Barry, Bridgette A.; “*In vivo, In vitro*, and Calculated Vibrational Spectra of Plastoquinone and Plastoquinone Anion Radical”; *J. Phys. Chem. B* **1999**, *103*, 9790-9800.

44. Wise, Kristopher E.; Wheeler, R.A.; “Donor-Acceptor Assisted Diels-Alder Reaction of Anthracene and Tetracyanoethylene (TCNE)”; *J. Phys. Chem. A* **1999**, *103*, 8279-8287.

43. Grafton, Anthony Kurt; Wheeler, R.A.; “Amino Acid Protonation States Determine Binding Sites of the Secondary Ubiquinone and its Anion in the *Rhodobacter sphaeroides* Photosynthetic Reaction Center; *J. Phys. Chem. B* **1999**, *103*, 5380-5387.
Highlighted in NSF publicity magazine *Access* Fall/Winter 1998, pp. 41-43. Featured at the NSF/National Center for Supercomputing Application’s “ACCESS Center” adjacent to NSF headquarters in Washington DC.

42. Wise, Kristopher E.; Pate, J. Brett; Wheeler, R.A.; “Phenoxyl, (Methylthio)phenoxyl, and (Methylthio)cresyl Radical Models for the Structures, Vibrations, and Spin Properties of the Cysteine-Linked Tyrosyl Radical in Galactose Oxidase”; *J. Phys. Chem. B* **1999**, *103*, 4764-4772.

41. Skokov, Sergei; Wheeler, R.A.; "Oxidative Aromatic Substitution: Hartree-Fock/Density Functional and *Ab Initio* Molecular Orbital Studies of Benzene and Toluene Nitrosation"; *J. Phys. Chem. A* **1999**, *103*, 4261-4269.

40. Raymond, Kevin S.; Wheeler, R.A.; "Compatibility of Correlation-Consistent Basis Sets with the Becke3LYP Hybrid Hartree-Fock/Density Functional"; *J. Comput. Chem.* **1999**, *20*, 207-216.

39. Grafton, Anthony Kurt; Wheeler, R.A.; "Vibrational Projection Analysis: A New Tool for Comparing Normal Vibrational Modes of Similar Molecules"; *J. Comput. Chem.* **1998**, *19*, 1663-1674.

38. Grafton, Anthony Kurt; Wheeler, R.A.; "ViPA: A Computer Program for Vector Projection Analysis of Normal Vibrational Modes of Molecules"; *Comput. Phys. Commun.* **1998**; *113*, 78-84.

37. Boesch, Scott E.; Wheeler, R.A.; "π-Donor Substituent Effects on Calculated Structures, Spin Properties, and Vibrations of Radical Anions of p-Chloranil, p-Fluoranil, and p-Benzoquinone"; *J. Phys. Chem. A* **1997**, *101*, 8351-8359.

36. Grafton, Anthony Kurt; Wheeler, R.A.; "Comparison of the Properties of Various Fused-Ring Quinones and Their Radical Anions Using Hartree-Fock and Hybrid Hartree-Fock/Density Functional Methods"; *J. Phys. Chem. A* **1997**, *101*, 7154-7166.

35. Boesch, Scott E.; Wheeler, R.A.; "Structures and Properties of Ubiquinone-1 and its Radical Anion Predicted from a Hybrid Hartree-Fock/Density Functional Method"; *J. Phys. Chem. A* **1997**, *101*, 5799-5804.

34. Grafton, Anthony Kurt; Boesch, Scott E.; Wheeler, R.A.; "Structures and Properties of Vitamin K and its Radical Anion Predicted by Hybrid Hartree-Fock/Density Functional Theory"; *J. Mol. Struc. (Theochem)* **1997**, *392*, 1-11.

33. Skokov, Sergei; Wheeler, R.A.; "Study of Hydrogen Abstraction Reactions by Hybrid Hartree-Fock/Density Functional Methods"; *Chem. Phys. Lett.* **1997**, *271*, 251-258.

32. Walden, Susan E.; Wheeler, R.A.; "First Evidence of Anchimeric Spin Delocalization in Tryptophan Radical Cation"; *J. Am. Chem. Soc.* **1997**, *119*, 3175-3176.
Highlighted in Chemical & Engineering News, "Science/Technology Concentrates" for April 7, 1997, p. 49.

31. Wise, Kristopher E.; Grafton, Anthony Kurt; Wheeler, R.A.; "Trimethyl-p-Benzoquinone Provides Excellent Structural, Spectroscopic, and Thermochemical Models for Plastoquinone-1 and its Radical Anion"; *J. Phys. Chem. A* **1997**, *101*, 1160-1165.

30. Raymond, Kevin S.; Grafton, Anthony Kurt; Wheeler, R.A.; "Calculated One-Electron Reduction Potentials and Solvation Structures for Selected p-Benzoquinones in Water"; *J. Phys. Chem. B* **1997**, *101*, 623-631.

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21. Wheeler, R.A.; "A Method for Computing One-Electron Reduction Potentials and its Application to p-Benzoquinone in Water at 300 K"; *J. Am. Chem. Soc.* **1994**, *116*, 11048-11051.

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19. Huang, Weiwei; Frech, Roger; Wheeler, R.A.; "Molecular Structures and Normal Vibrations of $CF_3SO_3^-$ and its Lithium Ion Pairs and Aggregates"; *J. Phys. Chem.* **1994**, *98*, 100-110.

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7. Jørgensen, Karl-Anker; Wheeler, R.A.; Hoffmann, Roald; "Electronic and Steric Factors Determining the Asymmetric Epoxidation of Allylic Alcohols by Titanium-Tartrate Complexes (The Sharpless Epoxidation)". *J. Am. Chem. Soc.* **1987**, *109*, 3240-3246.

6. Chandrasekhar, P.; Wheeler, R.A.; Hoffmann, Roald; "Sigma Bond Cleavage in Coordinated Dioxygen: The Case of the μ-Peroxo Complex $[((THF)_3Cl_2V^{III})_2(\mu\text{-}O_2^{2-})]$ and Vanadyl Formation in Solution". *Inorg. Chim. Acta* **1987**, *122*, 51-59.

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Highlighted in *Nachrich. Chem., Technik, Lab.* Vol. 35, Number. 2, p. 109; **1987** (Significant Advances in Inorganic Chemistry for 1986).

4. Wheeler, R.A.; Hoffmann, Roald; Strähle, Joachim; "Transition Metal Nitrides, Organic Polyenes, and Phosphazenes: A Structural and Orbital Analogy" *J. Am. Chem. Soc.* **1986**, *108*, 5381-5387.

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2. Wheeler, R.A.; Whangbo, Myung-Hwan; Hughbanks, Timothy; Hoffmann, Roald; Burdett, Jeremy K.; Albright, Thomas A.; "Symmetric vs. Asymmetric Linear M-X-M Linkages in Molecules, Polymers, and Extended Networks" *J. Am. Chem. Soc.* **1986**, *108*, 2222-2236.

1. Wheeler, R.A.; Van Hecke, Gerald R.; "Application of Regular Solution Theory to Discotic Mesophases: Calculation of Phase Diagrams Exhibiting Minima" in *Liquid Crystals and Ordered Fluids*, vol. 4; A.C. Griffin, J.F. Johnson, eds.; Plenum: New York, **1984**; pp. 283-292.

EDITED VOLUMES:

9. *Annual Reports in Computational Chemistry*, Volume 10; R.A. Wheeler, ed.; Elsevier and ACS Computers in Chemistry Division: Amsterdam, 2014.

8. *Annual Reports in Computational Chemistry*, Volume 9; R.A. Wheeler, ed.; Elsevier and ACS Computers in Chemistry Division: Amsterdam, 2013.

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6. *Annual Reports in Computational Chemistry*, Volume 7; R.A. Wheeler, ed.; Elsevier and ACS Computers in Chemistry Division: Amsterdam, 2011.

5. *Annual Reports in Computational Chemistry*, Volume 6; R.A. Wheeler, ed.; Elsevier and ACS Computers in Chemistry Division: Amsterdam, 2010.

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2. *Annual Reports in Computational Chemistry*, Volume 3; D. Spellmeyer and R.A. Wheeler, eds.; Elsevier and ACS Computers in Chemistry Division: Amsterdam, 2007.

1. *Protein Bioenergetics: Simulations of Electron, Proton, and Energy Transfer*; R. A. Wheeler, ed.; ACS Symposium Series: Washington, DC, 2004.

INVITED PRESENTATIONS

University of Oklahoma Department of Chemistry and Biochemistry; Norman, OK; November 14, 2023; “What room temperature ionic liquids teach us about the structure of liquids”.

Kansas State University Department of Chemistry; Manhattan, KS; November 13, 2023; “What room temperature ionic liquids teach us about the structure of liquids”.

Western Illinois University Department of Chemistry; Macomb, IL; September 9, 2022; “Disordered nanocrystallite model for the structures of ionic liquids”.

American Chemical Society 263rd National Meeting; Symposium in honor of J. Andrew McCammon’s 70th Birthday; San Diego, CA; March 20, 2022; “Disordered nanocrystallite model for the structures of ionic liquids”.

St. Norbert College Department of Physics; De Pere, WI; October 14, 2021; “Disordered nanocrystallite model for the structures of ionic liquids for battery electrolytes”.

Lawrence University Department of Chemistry; Appleton, WI; October 13, 2021; “Disordered nanocrystallite model for the structures of ionic liquids for battery electrolytes”.

American Chemical Society 258th National Meeting; San Diego, CA; August 26, 2019; “Quantitation and visualization of static structure factor peaks for a phosphonium-based ionic liquid”; ENFL 0116; Mackoy, Travis; Wheeler, R.A.

Coalition for National Science Funding reception; Washington, DC; April 30, 2019 “BELONG in STEM: An educational partnership between Northern Illinois University and the NSF”; Wheeler, R.A.*; LaDue, N.; Hagen, T. (invited poster).

Argonne National Laboratory; Lemont, IL; April 10, 2019; “Temperature dependence of nanoscale ordering in a pyrrolidinium-based ionic liquid”.

North Central College; Department of Chemistry and Physics; Naperville, IL; April 1, 2019; “Temperature dependence of nanoscale ordering in a pyrrolidinium-based ionic liquid”.

Western Illinois University; Department of Chemistry; Macomb, IL; January 26, 2018; “Protonation states of histidine ligands to the oxidized Rieske iron-sulfur cluster of cytochrome bc1: Implications for coupled electron and proton transfer”.

Guangdong Medical University; Dongguang and Zhanjiang campuses, Guangdong Province, People’s Republic of China; December 29, 2017; “Functions of radicals important in energy storage by the photosynthetic reaction center and respiratory energy use by cytochrome bc1”.

Guangdong Medical University; Dongguang and Zhanjiang campuses; Guangdong Province, People’s Republic of China; December 28, 2017; “Organization of a typical American university”.

Northern Illinois University; Department of Computer Science; DeKalb, IL; October 31, 2016; “Computational chemistry: A personal perspective”.

Westminster College; Division of Science; New Wilmington, PA; March 18, 2016; “Protonation states of the histidine ligands to the oxidized Rieske iron-sulfur cluster of cytochrome bc1: Implications for coupled electron and proton transfer”.

Northern Illinois University; Department of Chemistry and Biochemistry; DeKalb, IL; January 28, 2016; “Protonation states of the histidine ligands to the oxidized Rieske iron-sulfur cluster of cytochrome bc1: Implications for coupled electron and proton transfer”.

South Dakota State University; Department of Chemistry and Biochemistry; Brookings, SD; January 22, 2016; “Protonation states of the histidine ligands to the oxidized Rieske iron-sulfur cluster of cytochrome bc1: Implications for coupled electron and proton transfer”.

Slippery Rock University; Department of Chemistry; Slippery Rock, PA; November 6, 2015; “How physics and chemistry conspire to explain biology and materials”.

11th Annual Metals in Biology Symposium; Duquesne University; Pittsburgh, PA; September 25, 2015; “^{15}N isotopic substitution distinguishes a protonated vs. deprotonated His ligand to the iron-sulfur cluster in human mitoNEET”; Ashlyn M. Koval, Benjamin R. Jagger, and R.A. Wheeler.

12th Annual MERCURY Conference on Undergraduate Computational Chemistry; Bucknell University; Lewisburg, PA; July 26, 2013; “Estimating free energy differences using molecular dynamics simulations: Amino acid side chain pK_a values in cytochrome bc_1”.

Carnegie-Mellon University; Department of Chemistry; Pittsburgh, PA; October 6, 2011;”Amino acid side chain protonation states and their role in cofactor binding in the electron transfer protein cytchrome bc1”.

Saint Francis University; Department of Chemistry; Loretto, PA; September 23, 2011; “Amino acid side chain pKa values and ubiquinol binding sites in cytochrome bc_1”.

Duquesne University; Department of Chemistry & Biochemistry; Pittsburgh, PA; January 11, 2010; “Ab initio computer simulations of protein folding”.

Washburn University; Department of Chemistry; Topeka, KS; October 15, 2009 “Ab initio computer simulations of protein folding”.

Oklahoma State University; Department of Chemistry; Stillwater, OK; February 7, 2008; “Ab initio computer simulations of protein folding”.

University of California-San Diego/Scripps Research Institute; Center for Theoretical Biological Physics; March 3, 2006; “Principal mode analysis: A new way to analyze molecular vibrations”.

University of California-Davis, Department of Chemistry; Davis, CA; November 15, 2005; “Molecular origami: folding proteins with a computer”.

Universidade Federal Fluminense, Departamento de Quimica; Rio de Janeiro, Brazil; June, 2005; “Principal mode analysis: A new way to understand molecular vibrations from dynamics simulations”.

Harvey Mudd College, Department of Chemistry; Claremont, CA; March 10, 2005; “Principal mode analysis: A new way to analyze molecular vibrations”.

University of California-Irvine, Department of Chemistry; Irvine, CA; March 8, 2005; “Principal mode analysis: A new way to analyze molecular vibrations”.

American Chemical Society Wichita Falls Local Section Meeting; Duncan, OK; October 19, 2004; “Molecular Origami: Folding Proteins with a Computer”.

Cameron University, Department of Chemistry; Lawton, OK; October 19, 2004; “Molecular Origami: Folding Proteins with a Computer”.

Southwestern Oklahoma State University, Department of Chemistry; Weatherford, OK; October 14, 2004; “Molecular Origami: Folding Proteins with a Computer”.

American Chemical Society 60th Southwest Regional Meeting; Ft. Worth, TX; September 29, 2004; “Principal Mode Analysis: Optimal Vibrational Spectra from Quantum or QM/MM Trajectories”.

Universidade Federal de Pernambuco, Departamento Quimica Fundamental; Recife, Brazil; March 18, 2004; “Role of Protein Conformations in Photosynthetic Electron Transfer”.

Universidade Estadual de Campinas, Departamento de Quimica; Campinas, Brazil; March 16, 2004; “Role of Protein Conformations in Photosynthetic Electron Transfer”.

Universidade Federal Fluminense, Departamento de Quimica; Rio de Janeiro, Brazil; March 10, 2004; “Role of Protein Conformations in Photosynthetic Electron Transfer”.

American Chemical Society 226th National Meeting; New York, NY; September 9, 2003; “Mining Molecular Dynamics Data for Molecular Properties” (one of 7 submissions selected from more than 30 applications to present in a special “Emerging Technologies” symposium).

Gordon Research Conference (Photosynthesis); Bristol, RI; June 27, 2003; “Protein Conformational Gating of Secondary Ubiquinone Binding in the *Rhodobacter Sphaeroides* Photosynthetic Reaction Center”.

American Chemical Society 225th National Meeting; New Orleans, LA; March 24, 2003; “Identifying a Potential Conformational Gate for Ubiquinone-B Binding in the Photosynthetic Reaction Center”; S.E. Walden and R.A. Wheeler.

University of North Texas, Department of Chemistry; Denton, TX; March 14, 2003; “Conformational Gating of Secondary Ubiquinone Binding in the *Rhodobacter Sphaeroides* Photosynthetic Reaction Center”.

Georgetown University, Department of Chemistry; Washington, DC; January 13, 2003; “Role of Protein Conformations in Photosynthetic Electron Transfer”.

University of Memphis, Department of Chemistry; Memphis, TN; October 18, 2002; “Role of Protein Conformations in Photosynthetic Electron Transfer”; R.A. Wheeler and S.E. Walden.

American Chemical Society 223rd National Meeting/Enhanced Sampling Techniques in Molecular Dynamics Simulations symposium; April 7, 2002; “Rigorous Classical-Mechanical Derivation of a Multiple-Copy Algorithm for Sampling Statistical Mechanical Ensembles”; R.A. Wheeler and C. Adam Hixson.

Southwestern Oklahoma State University, Department of Chemistry; Weatherford, OK; November 8, 2001; “How Photosynthesis Works”; R.A. Wheeler and S.E. Walden.

Lyon College, Department of Chemistry; Batesville, AR; October 8, 2001; “Protein Conformations and their Role in Photosynthesis”; S.E. Walden and R.A. Wheeler.

Arkansas State University, Department of Chemistry; Jonesboro, AR; October 5, 2001; “Protein Conformations and their Role in Photosynthesis”; S.E. Walden and R.A. Wheeler.

University of Missouri-Kansas City, Department of Chemistry; Kansas City, MO; November 2, 2000; “Computational Modeling of Quinone Reduction in Photosynthesis”.

Central Missouri State University, Department of Chemistry; Warrensburg, MO; November 1, 2000; “Computational Modeling of Quinone Reduction in Photosynthesis”.

University of Missouri-Columbia, Department of Chemistry; Columbia, MO; October 31, 2000; “Computational Modeling of Quinone Reduction in Photosynthesis”.

1st International Conference on Porphyrins and Phthalocyanines”; Dijon, France; June 30, 2000; “Electronic Structure of Nitrosyl Metalloporphyrins”;. R. A. Wheeler, C. Adam Hixson.

Kwangju Institute of Science and Technology, Department of Materials Science and Engineering; Kwangju, Korea; May 23, 2000; “Molecular Dynamics Simulations of Tetraglyme/MCF_3SO_3 (M = Na, Li) Melts: Structural and Conformational Properties”. Jin-Kee Hyun and R. A. Wheeler.

Chungbuk National University, Department of Chemistry; Chungbuk, Korea; May 18, 2000; “Molecular Dynamics Simulations of Tetraglyme/MCF_3SO_3 (M = Na, Li) Melts: Structural and Conformational Properties”. Jin-Kee Hyun and R. A. Wheeler.

Korea Research Institute of Chemical Technology; Advanced Materials Division; Taejon, Korea; May 17, 2000; “Molecular Dynamics Simulations of Tetraglyme/MCF_3SO_3 (M = Na, Li) Melts: Structural and Conformational Properties”. Jin-Kee Hyun and R. A. Wheeler.

Kansas State University, Department of Biochemistry; Manhattan, KS; December 6, 1999; “Energetics of Quinone Binding in Photosynthesis”.

Albuquerque High Performance Computing Center/University of New Mexico; Albuquerque, NM; October 6, 1999; “Energetics of Quinone Binding in Photosynthesis”.

OCAST Health Research Conference; Oklahoma City, OK; September 21, 1999; “Quinone Binding and Reduction in Photosynthesis”; R. A. Wheeler.

American Chemical Society 217th National Meeting/Bioenergetics Symposium; New Orleans, LA; August 24, 1999; “Structural, Thermochemical, and Binding Properties of Quinones and

Their Anions in the Photosynthetic Reaction Center of *Rhodobacter sphaeroides*"; R.A. Wheeler.

23rd Department of Energy Solar Photochemistry Conference; Tahoe City, CA; June 9, 1999; "Quinone Binding and Reduction in the Photosynthetic Reaction Center"; R. A. Wheeler.

Oklahoma State University, Department of Chemistry; Stillwater, OK; February 18, 1999; "Donor-Acceptor-Assisted Diels-Alder Reactions".

22nd Department of Energy Solar Photochemistry Conference; June 9, 1998;Chantilly, VA; "Calculated Binding Sites of the Secondary Quinone Q_B and Q_B^- in the Photosynthetic Reaction Center from *Rhodobacter sphaeroides*"; R. A. Wheeler, A. K. Grafton (poster).

University of California; San Francisco, CA; June 2, 1998; "Calculated Binding Sites for the Secondary Quinone Q_B and Q_B^- in the Photosynthetic Reaction Center from *Rhodobacter sphaeroides*".

American Chemical Society 215th National Meeting/Electron Transfer Symposium; Dallas, TX; April 2, 1998; "*Ab Initio* Molecular Orbital/Molecular Dynamics Simulations of Electron Transfer"; R. A. Wheeler, S. Skokov.

American Chemical Society 215th National Meeting/Organic Reactions Symposium; Dallas, TX; March 30, 1998; "Electrophilic vs. Oxidative Aromatic Substitutions: Hartree-Fock/Density Functional Studies of Benzene and Toluene Nitration and Nitrosation"; R. A. Wheeler, S. Skokov.

University of California; San Francisco, CA; November 13, 1997; "First *Ab Initio* Molecular Dynamics Simulation of Electron Transfer".

American Chemical Society 213th National Meeting/Recent Developments in Molecular Simulations Using Density-Functional Theory Symposium; San Francisco, CA; April 16, 1997; "Study of Hydrogen Abstraction Reactions by Hartree-Fock/Density Functional Methods"; S. Skokov, R. A. Wheeler;

American Chemical Society 213th National Meeting/Frontiers of Electronic Structure Theory Symposium; San Francisco, CA; April 14, 1997; "First Evidence of Anchimeric Spin Delocalization in Tryptophan Radical Cation"; S. E. Walden, R. A. Wheeler.

American Chemical Society 209th National Meeting/Physical Chemistry of Proteins Symposium; Anaheim, CA; 3 April 1995; "Phenoxyl vs. Tyrosine Phenoxyl Radical Structures, Vibrations, and Spin Densities"; Y. Qin, R. A. Wheeler.

Arkansas State University, Department of Chemistry; Jonesboro, AR; March 14, 1995; "Predicting Properties of Amino Acid Radicals Implicated in Cancer and Aging".

Wichita State University, Department of Chemistry; Wichita, KS; January 25, 1995; "Toward the Computer-Aided Design of Molecular Redox Properties".

American Chemical Society 50th Southwest Regional Meeting; Ft. Worth, TX; November 14, 1994; "Computer-Assisted Modeling of Quinone Electrochemistry in Water at 300K".

American Chemical Society 29th Midwest Regional Meeting; Kansas City, MO; November 4, 1994; "Semi-Empirical vs. *Ab Initio* Computation of Structures, Vibrational Frequencies, and Energies for Tetra-Substituted *p*-Benzoquinones and Their Radical Anions" (with S.E. Boesch).

University of Warsaw, Quantum Chemistry Laboratory, Department of Chemistry; Warsaw, Poland; May 26, 1993; "Structure, Bonding, and Hydration of *p*-Benzoquinone and *p*-Benzosemiquinone Anion".

Russian Academy of Sciences, Institute of Physical Chemistry; Moscow, Russia; May 22, 1993; "The Inert Pair Effect in Group 15 Halides".

Eidgenössische Technische Hochschule (ETH Zentrum), Laboratorium für Physikalische Chemie; Zürich, Switzerland; May 19, 1993; "Structure, Bonding, and Hydration of *p*-Benzoquinone and *p*-Benzosemiquinone Anion".

Freie Universität Berlin, Institut für Anorganische und Analytische Chemie; Berlin, Germany; May 14, 1993; "The Inert Pair Effect in Group 15 Halides".

Technische Universität Berlin, Institut für Anorganische und Analytische Chemie; Berlin, Germany; May 12, 1993; "The Inert Pair Effect in Group 15 Halides".

University of Missouri-Kansas City, Department of Chemistry; Kansas City, MO; March 26, 1992; "Stereochemically Active or Inactive Lone-Pair Electrons in Some Six-Coordinate, Group 15 Halides".

Oklahoma State University, Department of Chemistry; Stillwater, OK; February 13, 1992; "Stereochemically Active or Inactive Lone-Pair Electrons in Some Six-Coordinate, Group 15 Halides".

Texas Lutheran College, Department of Chemistry; Sequin, TX; November 8, 1991; "Stereochemically Active or Inactive Lone-Pair Electrons in Some Six-Coordinate, Group 15 Halides".

Pittsburg State University, Department of Chemistry; Pittsburg, KS; February 15, 1991; "Transition Metal Clusters as Pieces of Infinite Solids".

Northern Illinois University, Department of Chemistry; DeKalb, IL; January 31, 1989; "A Reciprocal Space Approach to the Orbitals of Finite Crystals".

Temple University, Department of Chemistry; Philadelphia, PA; January, 1988; "Cluster, Surface, and Interface Chemistry: A Reciprocal Space Approach to the Orbitals of Truncated Crystals".

Aarhus University, Department of Chemistry; Aarhus, Denmark; December, 1986; "Orbital Topology and Chemical Reactivity".

University of Stockholm, Institute for Theoretical Physics; Stockholm, Sweden; October, 1986; "Localized vs. Delocalized Bonding in Transition-Metal Nitride Chains and Rings".

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