

Weitao Yang

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Present Position and Address

Philip Handler Professor of Chemistry
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Research Interests

Physical Chemistry, Theoretical Chemistry, Electronic Structure Theory, Density Functional Theory, Biophysical Chemistry, Nano Science and Condensed Matters.

Personal

Born on March 31, 1961 in Chaozhou, China. U. S. citizen
Married, wife Helen Wen Yang, and two children.

Education

February 1978 - February 1982

BS degree in Chemistry, Peking University, Beijing China

August 1982 - September 1986

Ph.D. degree in Chemistry, under the direction of Professor Robert G. Parr, University of North Carolina, Chapel Hill.

Dissertation Title: "Studies in Density Functional Theory: Chemical Reactivity; Kinetic Energy"

Employment/Experience

July 2003 - Present

Philip Handler Professor of Chemistry, Duke University

July 1999- June 2003

Professor, Department of Chemistry, Duke University

July 1995 - June 1999

Associate Professor, Department of Chemistry, Duke University

July 1989 - June 1995

Assistant Professor, Duke University

January 1988 - June 1989

Research Associate with Professor William H. Miller, Department of Chemistry, University of California, Berkeley

October 1986 - December 1987

Research Associate with Professor Robert G. Parr, University of North Carolina, Chapel Hill

Honors

2006-Elected Member of the International Academy of Quantum Molecular Science.

2006-Humboldt Research Award for Senior U.S. Scientists.

2005-Recognized by the Institute for Scientific Information as a Highly Cited Researcher, <http://isihighlycited.com/>

1999-2004-The Lee-Yang-Parr correlation energy functional, also known as the LYP functional (Phys. Rev. B 37, 785, 1988) has been the second most cited paper in chemistry for all six years from 1999 to 2004 since CAS started publishing citation data online: <http://www.cas.org/spotlight/bchem.html>

2005-Chang Jiang Visiting Professor, Tsinghua University, Beijing

2004-Visiting Professor, City University of Hong Kong

2003-Elected Fellow of American Association for the Advancement of Science

2003-Elected Fellow of American Physical Society

2003-Visiting Professor, Peking University

2000-2004-Overseas Assessor, Chinese Academy of Sciences

2000-Invitation Fellowship, Japanese Society for Promotion of Science

2000-Visiting Professor, Kyoto University

2000-Outstanding Overseas Chinese Young Scientist Award, Chinese National Science Foundation

1997-Annual Medal of the International Academy of Quantum Molecular Science

1996-1997-Visiting Associate Professor, The Hong Kong University of Science and Technology

1993- 1996-Sloan Research Fellow

1990 – 1991-The North Carolina Science and Engineering Award

1984 – 1985-The Award of Limited Service Assistantship, The Graduate School, University of North Carolina at Chapel Hill

1983-Dobbins Fellow, University of North Carolina at Chapel Hill

1981-Three-Merit Outstanding Student, Peking University

Editorial Board and Review Panel Service

NIH study section, Computational Biophysics-October 2005, February 2006, June 2006

External Advisory Committee, Department of Bioengineering, Rice University-, 2005-2006

NSF Site Review Panel, Purdue University-June 20-22, 2005

Executive Editor, Journal of Theoretical and Computational Chemistry, 2002-present

Associate Editor, Communications on Mathematical Sciences, 2002-present

Advisory Editor, Theoretical Chemistry Accounts, 1997-present

Advisory Editorial Board, the International Journal of Quantum Chemistry, 2002-present

Editorial Board, The Acta Physico-Chimica Sinica, 2000-present

Editorial Board, The Chinese Journal of Chemical Physics, 2002-present

Guest Editor, International Journal of Quantum Chemistry, 1997

NIH Special Emphasis Review Panel, Feb., 2002

NIH Special Emphasis Review Panel, Nov., 2002

DOE Review Panel, April, 2002

NSF Review Panel, Nov., 2001, Jun. 2005

Professional Fellowships and Memberships

Fellow of the American Association for the Advancement of Science

Fellow of the American Physical Society

Member of the American Chemical Society

Member of Sigma Xi

Symposium/Conference Organization

June 3-7, 1997 -Organizer, the Symposium on Density Functional Theory and Applications-A Satellite Symposium of the 9th International Congress of Quantum Chemistry, at Duke University.

November 12-17, 1997 -Co-organizer, with Dr. Juvencio Robles of the University of Guanajuato MEXICO the symposium on New Trends in Atomic and Molecular Structure Teaching at the Chemical Congress of North America, Cancun, Mexico.

November 5-6, 1998-Organizer, Quantum Chemistry Symposium in Honor of Robert G, Parr, the fiftieth Southeast Regional Meeting of the American Chemical Society, Research Triangle Park, North Carolina.

March 26-30, 2006-Organizer, "Frontier Applications and Developments of Density Functional Theory: A Symposium in Honor of Robert G. Parr's 85th Birthday", the 231st National Meeting of the American Chemical Society, March 26-30, 2006, Atlanta, Georgia.

Publications

- [1] R. G. Parr and W. Yang, "Density-functional approach to the frontier-electron theory of chemical reactivity," *J. Am. Chem. Soc.*, vol. 106, p. 4049, 1984.
- [2] W. Yang, R. G. Parr, and R. Pucci, "Electron density, kohn-sham frontier orbitals, and fukui functions," *J. Chem. Phys.*, vol. 81, p. 2862, 1984.
- [3] M. Levy, W. Yang, and R. G. Parr, "A new functional with homogeneous coordinate scaling in density-functional theory: $f[\rho, \lambda]$," *J. Chem. Phys.*, vol. 83, p. 2334, 1985.
- [4] W. Yang, C. Lee, and S. K. Ghosh, "Molecular softness as the average of atomic softnesses: Companion principle to the geometric mean principle for electronegativity equalization," *J. Phys. Chem.*, vol. 89, p. 5412, 1985.
- [5] W. Yang and R. G. Parr, "Hardness, softness, and fukui function in the electronic theory of metals and catalysis," *Proc. Natl. Acad. Sci. USA*, vol. 82, p. 6723, 1985.
- [6] W. Yang and J. E. Harriman, "Analysis of the kinetic energy functional in density-functional theory," *J. Chem. Phys.*, vol. 84, p. 3320, 1986.
- [7] W. Yang, "Gradient correction in thomas-fermi theory," *Phys. Rev. A*, vol. 34, p. 4575, 1986.
- [8] W. Yang, R. G. Parr, and C. Lee, "Various functionals for the kinetic energy density of an atom or molecule," *Phys. Rev. A*, vol. 34, p. 4586, 1986.
- [9] W. Yang and W. J. Mortier, "The use of global and local molecular parameters for the analysis of the gas-phase basicity of amines," *J. Am. Chem. Soc.*, vol. 108, p. 5708, 1986.
- [10] W. Xue and W. Yang, "Application of a scaled particle theory to polar solute system and calculation of the salt effect constant," *Acta Physico-Chimica Sinica*, vol. 3, p. 258, 1987.
- [11] W. Yang, "Ab initio approach for many-electron system without invoking orbitals: An integral formulation of density-functional theory," *Phys. Rev. Lett.*, vol. 59, p. 1569, 1987.
- [12] W. Yang, R. G. Parr, and L. Uytterhoeven, "New relation between hardness and compressibility of minerals," *Phys. and Chem. of Minerals*, vol. 15, p. 191, 1987.
- [13] W. Yang, "Some remarks on scaling relations in density-functional theory," in *Density Matrices and Density-Functionals* (R. Erdahl and J. V. H. Smith, eds.), pp. 499-506, Dordrecht, Holland: D. Reidel Publishing Company, 1987.
- [14] C. Lee, W. Yang, and R. G. Parr, "Local softness and chemical reactivity in the molecules CO , SCN , and HCO ," *Theochem*, vol. 163, pp. 305-313, 1988.

- [15] C. Lee, W. Yang, and R. G. Parr, "Development of the colle-salvetti correlation energy formula into a functional of the electron density," *Phys. Rev. B*, vol. 37, pp. 785-789, 1988.
- [16] W. Yang, "Ab initio approach for many-electron systems without invoking orbitals: An integral formulation of density-functional theory," *Phys. Rev. A*, vol. 38, p. 5494, 1988.
- [17] W. Yang, "Thermal properties of many-electron systems: An integral formulation of density-functional theory," *Phys. Rev. A*, vol. 38, p. 5504, 1988.
- [18] W. Yang, "Dynamic linear response of many-electron systems: An integral formulation of density-functional theory," *Phys. Rev. A*, vol. 38, p. 5512, 1988.
- [19] W. Yang and A. C. Peet, "The collocation method for bound solutions of the schroedinger equation," *Chem. Phys. Lett.*, vol. 153, p. 98, 1988.
- [20] R. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules*. New York: Oxford University Press, 1989.
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- [23] W. Yang and W. H. Miller, "Block lanczos approach combined with matrix continued fraction for the s-matrix kohn variational principle in quantum scattering," *J. Chem. Phys.*, vol. 91, p. 3504, 1989.
- [24] W. Yang, A. C. Peet, and W. H. Miller, "A collocation approach for quantum scattering based on the s-matrix version of the kohn variational principle," *J. Chem. Phys.*, vol. 91, p. 7537, 1989.
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- [27] W. Yang and A. C. Peet, "A method for calculating vibrational bound states by iterative solution of the collocation equations constructed from localized basis sets," *J. Chem. Phys.*, vol. 92, p. 522, 1990.
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[110] S.-H. Ke, H. U. Baranger, and W. Yang, "Molecular conductance: Chemical trends of anchoring groups," *J. Am. Chem. Soc.*, vol. 126, no. 48, pp. 15897-15904, 2004.

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[152] R. Liu, S.-H. Ke, W. Yang, and H. U. Baranger, "Cobaltocene as a spin filter," *J. Chem. Phys.*, 2006. submitted.

[153] D. Xiao, W. Yang, and D. N. Beratan, "Inverse molecular design in a molecular orbital framework," *J. Phys. Chem. B*, 2006. submitted.

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Books

- Robert G. Parr and Weitao Yang, *Density-Functional Theory of Atoms and Molecules*, Oxford University Press (1989).
- Weitao Yang, Mel Levy, and S. Trickey, ed., "Special issue: Symposium on density functional and applications (Part I of II)", *Int. J. Quantum Chem.*, 69 (1998).

Invited Presentations at Conferences

1. Invited Talk, the A. John Coleman Symposium, Queen's University, Kingston, Canada, 1985.
2. Invited Talk, Chemistry Department Short Course Program, University of North Carolina, Chapel Hill, 1986.
3. Invited Talk, Symposium in Honor of Ernest L. Eliel and Robert G. Parr, Chapel Hill, North
4. Invited Talk, "Recent Computational Advances in Density-Functional Theory", 4th Annual Symposium of the North Carolina Section of the American Chemical Society, North Carolina State University, 1990.

5. Invited Talk, "Density-Functional Theory of Large Molecules", Twentieth Southeastern Theoretical Chemistry Association Conference, Clemson University, 1991.
6. Invited Talk, "Direct Calculation of Electron Density in Density-Functional Theory", The Third Annual Workshop on Recent Developments in Electronic Structure Algorithms, Cornell University, 1991.
7. Invited Talk, "Direct Calculation of Electron Density: A Divide-and-Conquer Approach to Large Molecules", The VIIth International Congress of Quantum Chemistry, Menton, France, 1991.
8. Invited Talk, "Density-Functional Theory of Large Systems: a divide-and-conquer approach" XVIth International Workshop on Condensed-Matter Theories, San Juan, Puerto Rico, 1992.
9. Invited Talk, "Direct Calculation of Electron Density for Molecules and Solids", NSERC-CAP Summer Institute in Theoretical Physics, Workshop on Density-Functional Theory: Methods and Applications, Kingston, Canada, 1992.
10. Invited Talk, "Density Functional Approach to Large Molecules", 76th Canadian Society for Chemistry Conference and Exhibition, Sherbrooke, Canada, 1993.
11. Invited Talk, "Density-Functional Computation of Large Molecular Systems", The 1994 Society for Computer Simulation Multiconference, La Jolla, San Diego, California, April 9-4, 1994.
12. Invited Plenary Lecture, "A Divide-and-Conquer Method and Its Applications to Large Molecules", the 2nd Canadian Computational Chemistry Conference, Kingston, Ontario, Canada, May 21-25, 1994.
13. Invited Plenary Lecture, "Density-Functional Approach to Large Molecules", Satellite Symposium of the 8th International Congress of Quantum Chemistry: Thirty Years of Density-Functional Theory, Cracow, Poland, June 13-16, 1994.
14. Invited Serial Lectures, "Four Lectures on Density-Functional Theory", the 1994 International Seminar Series on Theoretical Chemistry Development, Nanjing University, Nanjing, China, June 24-July 3, 1994.
15. Invited Talk, "Theory and Applications of an $O(N)$ Method for Electronic Structure Calculations", Density-Functional Theory Research Program, the Institute of Theoretical Physics, University of California, Santa Barbara, California, July 5-29, 1994.
16. Invited Talk, "Theory and Applications of a Divide-and-Conquer Method for Large Molecules", in the International Workshop " Electronic Structure Methods for Truly Large Systems: Moving the Frontiers in Quantum Chemistry", Braunlage, Germany, August 1-7, 1994.
17. Invited Talk, "A Divide-and-Conquer Method and Its Application to the Modeling of Large Molecules on Parallel Computers", International Conference on Computing in Environmental Management, Raleigh, North Carolina, November 30-December 2, 1994.
18. Invited Talk, "A Divide-and-Conquer Density-Functional Approach for Large Molecules: Analytic energy Gradients and Geometry Optimization", The Thirty-Fifth Sanibel Symposium, St. Augustine, Florida, February 25 - March 4, 1995.

19. Invited Talk, "Density-Functional Approach for Large Molecules: Theory and Applications", 209th American Chemical Society National Meeting, Anaheim, California, April 2-6, 1995.
20. Invited Talk, "The Divide-and-Conquer Strategy for Linear Scaling Electronic Structure Calculations", CECAM Workshop on Linear Scaling Methods in Electronic Structure Theory, Lyon, France, July 5-7, 1995.
21. Invited Plenary Lecture, "Linear Scaling Methods for Electronic Structure Calculations: The Divide-and-Conquer Strategy", The 12th Canadian Symposium on Theoretical Chemistry, Fredericton, Canada, August 6-11, 1995.
22. Invited Talk, "The Divide-and-Conquer Density-Functional Approach for Large Molecules: Analytic Energy Gradients and Geometry Optimization", The First Conference for Worldwide Young Chinese Chemists", Beijing, China, August 20-24, 1995.
23. Invited Talk, "Linear Scaling Methods for Density-Functional Calculations", 6th International Conference on the Applications of Density-Functional Theory in Chemistry and Physics, Paris, France, August 29-September 1, 1995.
24. Invited Talk, "Linear Scaling Quantum Mechanical Studies of Biological Macromolecules in Solution", March Meeting of the American Physical Society, St. Louis, Missouri, March 18-22, 1996.
25. Invited Talk, "Towards Linear Scaling Computation for Large Molecules with Density-Functional Theory", The Second International Conference on Theoretical Chemical Physics, New Orleans, Louisiana, April 8-13, 1996.
26. Invited Talk, "Towards Linear Scaling Computation for Large Molecules with Density-Functional Theory", International Workshop on Density Functional Theory, Brisbane, Australia, July 14-20, 1996.
27. Invited Talk, "Describing Van der Waals Interactions with GGA ?", CECAM Workshop "Going Beyond the Local Density Approximation in Physics and Chemistry", Lyon, France, September 9-14, 1996.
28. Invited Talk, "Quantum Mechanical Study of Aqueous Polarization Effects in Biological Macromolecules", Symposium on Computational Structural Biology: Basics to Drug Design, University of North Carolina-Chapel Hill, February 25, 1997.
29. Invited Talk, "Absolute Energy Minimum Principles for Linear-Scaling Electronic Structure Calculations", Symposium on Density Functional Theory and Applications, A Satellite Symposium of the 9th International Congress of Quantum Chemistry, Durham, North Carolina, June 3-7, 1997.
30. Invited Talk, "Theory and Applications of Linear Scaling Electronic Structure Methods", the 9th International Congress of Quantum Chemistry, Atlanta, June 9-14, 1997.
31. Invited Talk, "New developments in $O(N)$ methods, divide-and-conquer approach to embedded calculations of solids and surfaces", CECAM Workshop "Reactivity at Surfaces", Lyon, France, August 28-30, 1997.
32. Invited Talk, "Quantum Mechanical Study of Macromolecules with a Continuum Model of Solvent", 214th American Chemical Society National Meeting, Las Vegas, Nevada, September 7-11, 1997.

33. Invited Talk, "Recent Development of Linear Scaling Quantum Mechanical Methods for Large Systems", 214th American Chemical Society National Meeting, Las Vegas, Nevada, September 7-11, 1997.
34. Invited Talk, "Density Functional Method for Large Systems: Theory and Application", the 5th Chemical Congress of North America, Cancun, Mexico, November 12-17, 1997.
35. Invited Talk, "Divide-And-Conquer Approach to the Simulation of Large Systems", the American Physical Society, Los Angeles, March 15-20, 1998.
36. Invited Talk, "Linear-Scaling Quantum Mechanical Methods and Applications", Gordon Research Conference on Computational Chemistry, Tilton, New Hampshire, June 28-July 3, 1998.
37. Invited Talk, "Linear Scaling Methods and Applications to Biological Systems", Cecam Workshop, Local Orbital Methods for Large Scale Atomistic Simulations, Lyon, France, July 22-25 1998.
38. Invited Talk, "Linear scaling methods and density functional theory", International Symposium on the Discrete Variational Method and Applications, Beijing and Chengdu, China, August 15-24, 1998.
39. Invited Talk, "Fractional Number of Electrons and Self-Interaction Error in Density Functional Theory", International Symposium on the Discrete Variational Method and Applications, Beijing and Chengdu, China, August 15-24, 1998.
40. Invited Plenary Talk, "Linear Scaling Quantum Mechanical Methods and Applications", The Thirty-Ninth Sanibel Symposium, St. Augustine, Florida, February 26 - March 5, 1999.
41. Invited Plenary Talk, "Linear Scaling Electronic Structure Methods and Applications to Biological Systems", The American Conference on Theoretical Chemistry, Boulder, Colorado, June 27-July 2, 1999.
42. Invited Talk, "Comparison Between Density Functional Theory and Density Matrix Theory", The Workshop on Reduced Density Matrix Theory, Kingston, Ontario, Canada, August 30-31, 1999.
43. Invited Talk, "Generate Ground States and Fractional Number of Electrons in Density Functional and Density Matrix Functional Theory", The Workshop on Reduced Density Matrix Theory, Kingston, Ontario, Canada, August 30-31, 1999.
44. Invited Talk, "Degenerate Ground States and Fractional Number of Electrons in Density and Reduced Density Matrix Functional Theory ", Satellite Symposium of the 10th International Congress of Quantum Chemistry, Menton, France, June 11-14, 2000.
45. Invited Talk, "How to Model Chemical Reactions in Enzymes ", International Chinese Workshop on Computational Chemistry, Dalian, China, August 14-19, 2000.
46. Invited Talk, "Free energy calculation of enzyme reactions with a DFT QM/MM method; application Enolase", Hawaii, PACIFICCHEM 2000, December, 2000.
47. Invited Talk, "Reaction Mechanism of Triosephosphate Isomerase: Is There a Low-Barrier Hydrogen Bond Involved ? A Theoretical Study with a QM/MM free energy method.", Structure Biology and Bioinformatics Conference, University of North Carolina at Chapel Hill, School of Medicine, March 8, 2001.

48. Invited Talk, "DFT QM/MM method for simulation of chemical reactions in enzymes", Chemical Dynamics Symposium in Honor of William H. Miller, The University of California, Berkeley, CA, March 28-31, 2001.
49. Invited Talk, "Computational studies of Enzymes and Proteins with Quantum Mechanical Methods", Southeast Theoretical Chemistry Association Annual Meeting, Auburn, Alabama, May 17-19, 2001.
50. Invited Talk, "Development and Applications of a DFT QM/MM Free Energy Method", CECAM International Workshop "New Methods For Combining Born-Oppenheimer Ab-Initio Calculations And Empirical Force Fields In Large Scale Simulation Studies", Lyon, France, June 13-15, 2001.
51. Invited Talk, "DFT QM/MM method for simulation of chemical reactions in enzymes", American Chemical Society National Meeting, Chicago, August 26-30, 2001.
52. Invited Talk, "Linear Scaling Approaches with the Divide-and-Conquer Method and with Localized Orbitals", CECAM International Workshop "Local orbitals and linear-scaling ab initio calculations", Lyon, France, September 3-7, 2001.
53. Invited Talk, "An Ab Initio QM/MM Free Energy Method For Simulating Enzyme Reaction Mechanisms And Its Application To Triosephosphate Isomerase", American Chemical Society Southeast Regional Meeting, Savannah, GA, September 23-26, 2001.
54. Invited Talk, "Computational Simulations of Enzymes and Proteins with Quantum Mechanical Methods: Development and Applications", Computational Chemistry GRID Conference, University of Kentucky, Lexington, Kentucky, October 16-17, 2001.
55. Invited Talk, "Quantum Mechanical Studies of Protein Dynamics and Functions", American Physical Society March Meeting, Indianapolis, March 18-22, 2002.
56. Invited Talk, "Linear Scaling Methods and Applications with the Divide-and-Conquer Method and with Localized Orbitals", Linear Scaling Electronic Structure Methods Workshop, Institute of Pure and Applied Mathematics (IPAM), University of California, Los Angeles, April 1-6, 2002.
57. Invited Talk, "Developments and applications of a DFT QM/MM free energy method for simulation of chemical reactions in enzymes", American Chemical Society National Meeting, Orlando, April 7-11, 2002.
58. Invited Talk, "A new method for calculating the exchange correlation potentials from functionals of orbitals and applications to optimized effective potentials in density functional theory", 85th Canadian Society for Chemistry (CSC) Conference and Exhibition, Vancouver, Canada, June 1-6, 2002.
59. Invited Talk, "Exchange-Correlation Potential", CECAM workshop on Exchange Correlation Functionals: Assessment and Prospects", Lyon, France, June 10-14, 2002.
60. Invited Talk, "Exchange-Correlation Potentials: A New Method for Calculating the Exchange Correlation Potentials from Functionals of Orbitals and for Performing Conventional Density Functional Calculations with Correct Long Range Potentials", Sandia National Laboratory Workshop on Quantum Mechanical Techniques: Exchange-Correlation Functional in Density Functional Theory, Albuquerque, New Mexico, August 14-16 2002.

61. Invited Talk, "Developments and applications of a DFT QM/MM free energy method for simulation of chemical reactions in enzymes", Second Worldwide Chinese Theoretical and Computational Chemistry Conference, Taipei, Taiwan, September 2-7, 2002.
62. Invited Talk, "Simulation of chemical reactions in enzymes with a DFT QM/MM free energy method", the Modeling and Simulation for Materials Workshop Institute of Pure and Applied Mathematics (IPAM), University of California, Los Angeles, November 19-22, 2002.
63. Invited Talk, "Simulation of chemical reactions in enzymes with a DFT QM/MM free energy method", the 2002 Triangle Biophysics Seminar, University of North Carolina, Chapel Hill, November 15-16, 2002.
64. Invited Talk, "Calculation of accurate exchange-correlation potentials for ground-state, excited-state, and time-dependent DFT", the 225th ACS National Meeting (Division of Computers in Chemistry), New Orleans, LA, March 23-27, 2003.
65. Invited Talk, "Iterative optimization approach to the calculation of orbital functionals in density functional theory", the 225th ACS National Meeting (Division of Physical Chemistry), New Orleans, LA, March 23-27, 2003.
66. Invited Talk, Invited Talk, "Theory and Computation of the Kohn-Sham Potentials", II International Applied Statistical Physics Molecular Engineering Conference, Puerto Vallarta, Mexico, August 25 - 29, 2003.
67. Invited Talk, "Simulation of chemical reactions in enzymes with a density functional theory QM/MM energy method", the 226th ACS National Meeting, New York, September 7-11, 2003.
68. Invited Talk, "Exploring the Space of the Kohn-Sham Potentials", The 10th International Congress on the Applications of Density Functional Theory in Chemistry and Physics, Brussels (Belgium), September 7-12, 2003.
69. Invited Talk, "(1) O(N) Electronic Structure Calculations with Nonorthogonal Localized Molecular Orbitals (2) Distributed Computation of Reaction Paths in Enzymes", CECAM workshop "Component Architectures, Open Standards and Parallel Algorithms for Molecular and Atomistic Simulations on Large Grids, Supercomputers, Workstations and Clusters", Lyon, France, October 13-16, 2003.
70. Invited Talk, "Simulation of chemical reactions in enzymes with a density functional theory QM/MM energy method", International Symposium on Clusters and Nano-Assemblies: Physical and Biological Systems, Richmond, VA, November 10-13, 2003.
71. Invited Talk, "Simulation of Chemical Reactions in Enzymes with a DFT QM/MM free energy method", Sanibel Symposium, St. Augustine, Florida, February 29-March 5, 2004
72. Invited Talk, "Simulation of Chemical Reactions in Enzymes: Success and Challenge", Grid@Duke Conference, Durham, NC, April 13-14, 2004
73. Invited Talk, "Potential Functionals: Solution to the v -representability Problem and Theoretical Foundation for the Optimized Effective Potential in Density Functional Theory", the 16th Annual Workshop on Recent Developments in Electronic Structure Methods, Rutgers, the State University of New Jersey, New Brunswick, NJ, 27-30 May, 2004

74. Invited Talk, "(1) Potential functionals - dual to density functionals and solution to the v -representability problem. (2) Critical role of the hydrogen bond of a water molecule in the catalysis of 4-oxalocrotonate tautomerase.", The Nature of Hydrogen Bonding and Density Functional Theory", CECAM-PSI-K NETWORK WORKSHOP "The Nature of Hydrogen Bonding and Density Functional Theory", CECAM, Lyon, France 2-5 June 2004
75. Invited Talk, "Potential functionals: solution to the v -representability problem and theoretical foundation for the optimized effective potential in density functional theory". The 15th CANADIAN SYMPOSIUM ON THEORETICAL CHEMISTRY, Sainte-Adèle, Québec, Canada July 10-14, 2004
76. Invited Talk, "Simulation of nano and biological systems with linear scaling and multi-scale approaches", the Abdus Salam International Center for Theoretical Physics-NSFC-ICTS Asian/Pacific Regional School on: "Electronic Structure Methods and Their Applications" July 19 -30, 2004, Institute of Physics, Beijing, P.R. China
77. Invited Talk, "Potential functionals and orbital functionals in density functional theory" the Abdus Salam International Center for Theoretical Physics-NSFC-ICTS Asian/Pacific Regional School on: "Electronic Structure Methods and Their Applications" July 19 -30, 2004, Institute of Physics, Beijing, P.R. China
78. Invited Talk, "Simulation of nano and biological systems with linear scaling and multi-scale approaches", The Summer School on Computational Chemistry, Peking University, Beijing, China, August 1-20, 2004
79. Invited Talk, "Potential functionals and orbital functionals in density functional theory" The Summer School on Computational Chemistry, Peking University, Beijing, China, August 1-20, 2004.
80. Invited Talk, "Reaction path potential for simulation of chemical reactions in enzymes derived from ab initio QM/MM calculations", the symposium "Quantum/Classical Calculations in Chemistry and Biophysics" at the ACS National Meeting in Philadelphia, PA August 22-26, 2004.
81. Invited Talk, "Simulation of Biological Systems with Linear-Scale and Multi-Scale Approaches", Triangle Biophysics Symposium "Electrons to Proteins: Coupling and Linkage in Biology", NORTH CAROLINA BIOTECHNOLOGY CENTER, Research Triangle Park, NC, November 3-5, 2004
82. Invited Talk, "Simulation of Biological Systems with Linear-Scale and Multi-Scale Approaches", Computational and Theoretical Biology Symposium, Rice University, Houston, December 10-12, 2004
83. Invited Keynote Speech, "Simulations of nano and biological systems", International Workshop on Theoretical and Computational Chemistry of Complex Systems in conjunction with 3rd Chinese Theoretical and Computational Chemistry Conference, Hong Kong University of Science and Technology, January 3-7, 2005
84. Invited Talk, "Simulation of Structures and Functions of Proteins with Linear-scale and Multi-scale Approaches", Symposium on Quantitative Biology and Modeling joint with and Science at the Edge Seminar, Michigan State University, April 29, 2005

85. Invited Talk, "Potential and Orbital Functionals: Going beyond the Exact Exchange and towards van der Waals Interactions", CECAM Workshop: VAN DER WAALS FORCES AND DENSITY FUNCTIONAL THEORY, Lyon, France, June 13-17, 2005.
86. Invited Opening Lecture, "Simulation of chemical reaction in enzyme with the first-principles QM/MM free energy method", Southeastern Theoretical Chemistry Association Meeting 2005, University of Tennessee, Knoxville, June 17- 19, 2005
87. Invited Talk, "Potential and Orbital Functionals: Correlation Energy and Analytic Energy Gradients for OEP", Fifth Congress of the International Society for Theoretical Chemical Physics, New Orleans, Louisiana, July 20-26, 2005
88. Invited Talk, "Simulation of biomolecular systems with linear-scaling and multi-scale methods", The 40th IUPAC (International Union of Pure and Applied Chemistry) Congress, Innovation in Chemistry, Beijing, China, August 14-19, 2005
89. Invited Talk, "Simulation of chemical reactions in enzyme with the first-principles QM/MM free energy method", Workshop on Theoretical and Computational Biology, Institute of High Energy Physics, Chinese National Academy of Sciences, Beijing, China, August 23-26, 2005
90. Invited Talk, "Going beyond B3LYP: Self-interaction free exchange-correlation energy functional for thermodynamics and kinetics", Workshop on Theoretical and Computational Biology, Institute of High Energy Physics, Chinese National Academy of Sciences, Beijing, China, August 23-26, 2005
91. Invited Talk, "Development and application of methods for determining reaction paths in enzymatic reactions ", American Chemical Society National Meeting, Washington D.C., August 28-September 1, 2005
92. Invited Talk, "Going beyond B3LYP: Self-interaction free exchange-correlation energy functional for thermodynamics and kinetics", The 9th National Symposium on Quantum Chemistry, Guilin, China, October 10-12, 2005
93. Invited Talk, "Potential and Orbital Functionals: Analytic Energy Gradients for OEP and Self-Interaction-Free Exchange-Correlation Energy Functional for Thermochemistry and Kinetics", International Conference of Computational Methods in Sciences and Engineering, Loutraki, Korinthos, Greece, October 21-26, 2005
94. Invited Talk, "Reaction path potential for complex biomolecular systems derived from mixed QM/MM methods", March Meeting of American Physical Society, Baltimore, March 13-17, 2006
95. Invited Talk, "Self-interaction-free exchange-correlation functionals for thermodynamics and kinetics", International Symposium on "Quantitative Quantum Chemistry," in honor of Dr. Thom Dunning, Santa Fe, New Mexico, March 17-20, 2006
96. Invited Talk, "Self-interaction-free exchange-correlation functionals for thermodynamics and kinetics", the XIIth International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006

97. Invited Talk, "Designing Molecules by Optimizing Potentials", the Ab Initio Methods Symposium, the Canadian Society of Chemistry 2006 Conference, Halifax, Nova Scotia, May 27-31, 2006
98. Invited Talk, "Simulations of Complex Biological Systems with Quantum Mechanics and Statistical Mechanics", the Sixth Canadian Computational Chemistry Conference (CCCC6), the University of British Columbia, Vancouver, Canada, July 26-30, 2006
99. Invited Plenary Lecture, "Designing molecules by optimizing potentials", The 4th world-wide Chinese Theoretical and Computational Chemistry Conference (WCTCC), Kunming, China, August 6-10, 2006
100. Invited Talk, "Building Self-Interaction-Free Exchange-Correlation Functionals from the Adiabatic Connection", the International Workshop: "Density functional theory meets strong correlation", the Montauk Yacht Club, Long Island, New York, September 5-8, 2006
101. Invited Talk, "Simulations of Biological Systems with DFTB and the Divide-and-Conquer Linear Scaling Method", Symposium - DFTB, An Approximate DFT Method: Theory and Applications, Sponsored by Elsevier, National ACS Meeting in San Francisco, California, September 10-14, 2006
102. Invited Talk, "Free Energies of Chemical Reactions in Enzymes and Solutions: From Quantum Mechanics to Statistical Mechanics", Symposium - "Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory", National ACS Meeting in San Francisco, California, September 10-14, 2006
103. Invited Talk, "Simulations of Complex Biological Systems with Quantum Mechanics and Statistical Mechanics", Midwest Quantitative Biology Conference, Mission Point Resort, Mackinac Island, Michigan. September 29-October 1, 2006
104. Invited Talk, "Potential and Spin-Potential Functional Formalisms", Symposium on "Recent Advances in Density Functional and Applications", 62nd ACS Southwest Regional Meeting, Houston, Texas, October 19-22 2006
105. Invited Talk, "Optimized effective Potentials", Oberwolfach Workshop Mathematical and Numerical Aspects of Quantum Chemistry Problems", Oberwolfach, Germany, October 22-28, 2006

Invited Presentations at Institutions

1. Invited Talk, University of California, Irvine, 1987.
2. Invited Talk, Duke University, 1987.
3. Invited Talk, Rice University, 1987.
4. Invited Talk, Florida State University, 1988.
5. Invited Talk, University of California-Los Angeles, 1988.
6. Invited Talk, Hunter College, City University of New York, 1988.
7. Invited Talk, University of Arizona, 1988.
8. Invited Talk, "Density-Functional Theory of Large Molecules: A Divide-and-Conquer Approach", Department of Chemistry, East Carolina University, 1990.
9. Invited Talk, "Parallel Computation of Molecular Structure", The North Carolina Supercomputing Center, 1991.

10. Invited Talk, "Direct Calculation of Electron Density: A Divide-and-Conquer Approach to Large Systems", Condensed Matter Seminar, Department of Physics, Duke University, 1991.
11. Invited Talk, "Density-Functional Theory of Large Molecules: A Divide-and-Conquer Approach". Physical Chemistry Seminar, Department of Chemistry, University of North Carolina, Chapel Hill, 1992.
12. Invited Talk, "Practical Computational Schemes in Density Functional Theory", The North Carolina Supercomputing Center, 1992.
13. Invited Talk, "A Divide-and-Conquer Approach to Large Systems", Condensed-Matter Seminar, Department of Physics, University of North Carolina, Chapel Hill, 1992.
14. Invited Talk, "Implementation and Application of Density Functional Theory", School of Pharmacy, University of North Carolina, Chapel Hill, 1992.
15. Invited Talk, "Structure and Energies of Bucky Onions", Stacie Institute of Molecular Science, National Research Council, Canada, 1993
16. Invited Talk, "Structure and Energies of Bucky Onions", Hong Kong University of Science and Technology, Hong Kong, 1993.
17. Invited Talk, "Density Functional Approach to Large Molecules: the Shape of Bucky Onions""", Peking Univeristy, Beijing, China, 1993.
18. Invited Talk, "Density-Functional Theory of Large Systems", Sandia National Laboratories, Albuquerque, New Mexico, 1993.
19. Invited Talk, "A Divide-and-Conquer Method for Large Molecules: the Shape of Bucky Onions", Physical Chemistry Seminar, The University of Maryland, College Park, 1993.
20. Invited Talk, "A Divide-and-Conquer Density-Functional Approach and its Application to the Study of Bucky Onions", Chemistry Department Seminar, Tulane University, New Orleans, April 23, 1994.
21. Invited Talk, "A Divide-and-Conquer Method for Large Systems and its Application to the Studies of the Structure and Energetics of Bucky Onions", Chemistry Department Seminar, Duke University, Durham, North Carolina, September 9, 1994.
22. Invited Talk, "A Divide-and-Conquer Method and Its Application to Large Molecules", in the Workshop on Algorithms for Macromolecular Modeling, Kansas Institute for Theoretical and Computational Science, Lawrence, Kansas, September 30-October 2, 1994.
23. Invited Talk, "A Divide-and-Conquer Method and Its Application to Large Molecules", Physical Chemistry Seminar, University of Utah, Salt Lake City, October 10, 1994.
24. Invited Talk, "Density Functional Theory and Order N Methods", Molecular Dynamics Seminar, North Carolina Supercomputing Center, October 27, 1994.
25. Invited Talk, "Development and Applications of A Divide-and-Conquer Linear-Scaling Quantum Mechanical Computational Method for Macromolecules", The Kansas Center for Advanced Scientific Computing, Lawrence, Kansas, April 26, 1996.

26. Invited Talk, "Linear Scaling Quantum Mechanical Calculations for Macromolecules in Solution", The Department of Physics, Hong Kong University of Science and Technology, Kowloon, Hong Kong, October 10, 1996.
27. Invited Talk, "Linear-Scaling Quantum Mechanical Methods and Applications: Macromolecules in Solution", Tam Kang University, Taiwan, March 10, 1997.
28. Invited Talk, "Linear-Scaling Quantum Mechanical Methods and Applications: Macromolecules in Solution", National Chung-Cheng University, Chia-Yi, Taiwan, March 11, 1997.
29. Invited Talk, "Describing van der Waals Interaction in Diatomic Molecules with Generalized Gradient Approximations: the Role of the Exchange Functional", National Tsing-Hua University, Hsinchu, Taiwan, March 12, 1997.
30. Invited Talk, "Linear-Scaling Quantum Mechanical Methods and Applications: Macromolecules in Solution", National Tsing-Hua University, Hsinchu, Taiwan, March 13, 1997.
31. Invited Talk, "Linear-Scaling Quantum Mechanical Methods and Applications: Macromolecules in Solution", National Taiwan University and the Institute of Atomic and Molecular Sciences, Taipei, March 14, 1997.
32. Invited Talk, "Linear-Scaling Quantum Mechanical Methods and Applications: Macromolecules in Solution", Department of Chemistry, Hong Kong University, Hong Kong, March 19, 1997.
33. Invited Talk, "Linear-Scaling Quantum Mechanical Methods and Applications: Macromolecules in Solution", Department of Chemistry, Hong Kong University of Science and Technology, Hong Kong, April 3, 1997.
34. Invited Talk, "Linear-Scaling Quantum Mechanical Methods and Applications to Macromolecules in Solution", Department of Chemistry, University of Pittsburgh, Pittsburgh, December 4, 1997.
35. Invited Talk, "Density Functional Theory and Linear-Scaling Methods", Department of Chemistry, Peking University, Beijing, August 17, 1998.
36. Invited Talk, "Density Functional Theory and Applications", Department of Chemistry, Beijing Normal University, Beijing, August 19, 1998.
37. Invited Talk, "Fractional Number of Electrons and Self-Interaction Error in Density Functional Theory", Institute of Solid State Physics, Chinese Academy of Sciences, Hefei, August 25, 1998.
38. Invited Talk, "Linear-Scaling Quantum Mechanical Methods and Applications to Biological Macromolecules", Department of Biology, University of Science and Technology of China, Hefei, August 26, 1998.
39. Invited Talk, "Linear Scaling Quantum Mechanical Computation Methods", Department of Computer Science, Duke University, October 2, 1998.
40. Invited Talk, "Linear Scaling Quantum Mechanical Methods and Applications to Biological Macromolecules", Physics Colloquium, University of Louisville, Kentucky, October 16, 1998.
41. Invited Talk, "A Pseudo-Bond Approach To Combining Quantum Mechanical And Molecular Mechanical Methods", Quantum Theory Project, University of Florida, Gainesville, FL, December 9, 1998.
42. Invited Talk, "Quantum Mechanical Studies of Proteins and Enzymes", Department of Chemistry, University of Minnesota, Minneapolis, May 3, 1999.

43. Invited Talk, "Linear Scaling Quantum Mechanical Methods and Applications to Biological Macromolecules ", Department of Chemistry, University of Guannajuato, Mexico, May 3, 1999.
44. Invited Talk, "A Pseudo-Bond Approach To Combining Quantum Mechanical And Molecualr Mechanical Methods ", Department of Chemistry, University of Guannajuato, Mexico, May 3, 1999.
45. Invited Talk, "Quantum Mechanical Studies of Proteins and Enzymes", Biophysics Seminar, Duke University, Durham, September 13, 1999.
46. Invited Talk, "Degenerate Ground States and Fractional Numbers of Electrons in Density and Reduced Density Matrix Functional Theory ", Department of Synthetic and Biological Chemistry, Kyoto University, Kyoto, September 18, 2000.
47. Invited Talk, "Nonothogonal Localized Molecular Orbitals ", Department of Synthetic and Biological Chemistry, Kyoto University, Kyoto, September 18, 2000.
48. Invited Talk, "Study of enzyme reaction mechanisms with a density functional theory QM/MM method; application to Enolase", Department of Synthetic and Biological Chemistry, Kyoto University, Kyoto, September 21, 2000.
49. Invited Talk, "Linear Scaling Electronic Structure Methods and Applications to Large Systems", Department of Engineering Physics, Kyoto University, Kyoto, October 3, 2000.
50. Invited Talk, "Degenerate Ground States and Fractional Numbers of Electrons in Density and Reduced Density Matrix Functional Theory ", Department of Applied Chemistry, Tokyo University, Tokyo, October 10, 2000.
51. Invited Talk, "Free energy calculation of enzyme reactions with a DFT QM/MM method; application to Enolase", Department of Chemistry, The State University of New Jersey, Rutgers, Piscataway, December 12, 2000.
52. Invited Talk, "Computational studies of Enzymes and Proteins with Quantum Mechanical Methods", Department of Chemistry, University of Florida, Gainesville, FL, February 14, 2001.
53. Invited Talk, "Computational studies of Enzymes and Proteins with Quantum Mechanical Methods", Department of Chemistry, Indiana University, Bloomington, IN, April 12, 2001.
54. Invited Talk, "Development of a DFT QM/MM free energy method for enzyme reactions and application to enolase", Department of Chemistry, University of Arkansas, Fayetteville, AR, September 17, 2001.
55. Invited Talk, "Computater Simulations of Enzymes and Proteins with Quantum Mechanical Methods: Developemnt and Applications", Computational Chemistry GRID Conference, University of Kentucky, Lexington, Kentucky, October 16-17, 2001.
56. Invited Talk, "Developments and applications of a DFT QM/MM free energy method for simulation of chemical reactions in enzymes", Department of Chemistry, Purdue University, January 30, 2002.
57. Invited Talk, "Developments and applications of a DFT QM/MM free energy method for simulation of chemical reactions in enzymes", Department of Chemistry, Princeton University, February 14, 2002.

58. Invited Talk: "Direct method for optimized effective potentials in density functional theory", North Carolina Supercomputing Center, April 25, 2002.
59. Invited Talk, "Quantum Mechanical Studies of Protein Dynamics and Functions", Condensed Matter Seminar Series, Department of Physics, Duke University, May 2, 2002.
60. Invited Talk, "Developments and applications of a DFT QM/MM free energy method for simulation of chemical reactions in enzymes", School of Life Science, University of Science and Technology, Hefei, China, August 25, 2002.
61. Invited Talk, "Direct method for optimized effective potentials in density functional theory", Theoretical Chemistry Laboratory, Peking University, China, August 29, 2002.
62. Invited Talk, "Developments and applications of a DFT QM/MM free energy method for simulation of chemical reactions in enzymes", Stacy Institute, National Research Council, Ottawa, Canada, October 18, 2002.
63. Invited Talk, "Simulation of Chemical Reactions in Enzymes with a DFT QM/MM free energy method", Florida State University, January 22, 2003.
64. Invited Talk, "Simulation of Chemical Reactions in Enzymes with a DFT QM/MM free energy method", Ohio State University, January 28, 2003.
65. Invited Talk, "Simulation of Chemical Reactions in Enzymes with a DFT QM/MM free energy method", Old Dominion University, February 21, 2003.
66. Invited Talk, "Simulation of Chemical Reactions in Enzymes with a DFT QM/MM free energy method", Physical Chemistry Seminar, the University of North Carolina, Chapel Hill, April 23, 2003.
67. Invited Talk, "Exploring the Space of the Kohn-Sham Potentials", *Laboratoire de Chimie Théorique CNRS et Université Paris VI*, Paris, France, October 16, 2003.
68. Invited Talk, "Simulation of Chemical Reactions in Enzymes with a DFT QM/MM free energy method", Physical Chemistry Seminar, the University of Wisconsin, Madison, February 24, 2004
69. Invited Talk, "Simulation of Chemical Reactions in Enzymes with a DFT QM/MM free energy method", Physical Chemistry Seminar, Indiana University, Bloomington, February 6, 2004
70. Invited Talk, "Simulation of Chemical Reactions in Enzymes with a DFT QM/MM free energy method", Physical Chemistry Seminar, University of Notre Dame, April 15, 2004
71. Invited Talk, "Simulation of Chemical Reactions in Enzymes with a DFT QM/MM free energy method", Chemistry Departmental Seminar, Argonne National Laboratory, April 19, 2004
72. Invited Talk, "Simulation of Chemical Reactions in Enzymes with a DFT QM/MM free energy method", Seminar, Department of Chemical Engineering, North Carolina State University, April 27, 2004
73. Invited Talk, "Simulation of Chemical Reactions in Enzymes ", Hong Kong University of Science and Technology, Department of Chemistry, June 18, 2004
74. Invited Public Lecture, "Computer Simulations of Nano and Biological Systems", City University of Hong Kong, June 24, 2004

75. Invited Talk, "Simulation of nano and biological systems with linear scaling and multi-scale approaches", Seminar, Physics Department, Tsinghua University, July 23, 2004
76. Invited Departmental Colloquium, "Simulation of biological systems with linear-scale and multi-scale approaches", Department of Physics, Wake Forest University, November 11, 2004
77. Invited Talk, "Simulation of biological systems with linear-scale and multi-scale approaches", Department of Chemistry, Emory University, November 22, 2004
78. Invited Talk, "Development of potential and orbital functionals for accurate description of thermochemistry and kinetics", Department of Chemistry, The Pontificia Universidad Católica de Chile, Santiago, Chile, July 13, 2005
79. Invited Talk, "Going beyond B3LYP: Self-interaction free exchange-correlation energy functional for thermodynamics and kinetics", Department of Physics, Tsinghua University, Beijing, August 12, 2005
80. Invited Talk, "Advancing the frontiers of quantum mechanical simulation for complex biological systems and with higher accuracy", National Laboratory, University of Science and Technology, Hefei, August 19, 2005
81. Invited Talk, "Advancing the frontiers of quantum mechanical simulation for complex biological systems and with higher accuracy", Brook Haven National Laboratory, Upton, New York, November 9, 2005
82. Invited Talk, "Computer Simulation of Biological Systems with Linear-Scale and Multi-Scale Approaches", Laboratory of Structural, National Institute of Environmental Health, Research Triangle Park, North Carolina, December 1, 2005.
83. Invited Talk, Physics Colloquium, "Conductance Through Single Molecules: What Molecules Can Do and How Well Theory Describes it", Free University of Berlin, Berlin, June 16, 2007.
84. Invited Talk, Physical Chemistry Seminar, "Conductance Through Single Molecules: What Molecules Can Do and How Well Theory Describes it", University of Michigan, Ann Arbor, September 28, 2006

Invited Presentations Given by Other Group Members or Collaborator

1. Invited Talk, *Paula Mori-Sanchez*, Aron J. Cohen, Mel Levy, and Weitao Yang, "Development of exchange-correlation functionals from the adiabatic connection", Fifth Congress of the International Society for Theoretical Chemical Physics, New Orleans, Louisiana, July 20-26, 2005
2. Invited Talk, *Paula Mori-Sanchez*, Aron J. Cohen and Weitao Yang, "Development of exchange-correlation functionals from the adiabatic connection", Frontier Applications and Developments of Density Functional Theory: A Symposium in Honor of Robert G. Parr's 85th Birthday, the 231st National Meeting of the American Chemical Society, March 26-30, 2006, Atlanta, Georgia.

3. Invited Talk, *Aron Cohen*, Paula Mori-Sanchez and Weitao Yang, "Assessment of exchange correlation functionals from the adiabatic connection", Frontier Applications and Developments of Density Functional Theory: A Symposium in Honor of Robert G. Parr's 85th Birthday, the 231st National Meeting of the American Chemical Society, March 26-30, 2006, Atlanta, Georgia.
4. Invited Talk, *Mel Levy*, Aron Cohen, Paula Mori-Sanchez and Weitao Yang, "Early Days of DFT with RGP and a General Theory of Hybrids", Frontier Applications and Developments of Density Functional Theory: A Symposium in Honor of Robert G. Parr's 85th Birthday, the 231st National Meeting of the American Chemical Society, March 26-30, 2006, Atlanta, Georgia.
5. Invited Talk, *Hao Hu*, Jan Hermans and Weitao Yang, "Effective application of SCCDFTB in simulating structural and thermodynamic properties of molecular systems", Symposium - DFTB, An Approximate DFT Method: Theory and Applications, Sponsored by Elsevier, National ACS Meeting in San Francisco, California, September 10-14, 2006

Poster Presentations and Contributed Talks

1. Poster presentation, the Fifth American Conference on Theoretical Chemistry, Jackson, Wyoming, 1984.
2. Poster presentation, Chemical Dynamics Conference, Asilomar, California, 1989.
3. Poster Presentation, Chengteh Lee and Weitao Yang, "The Divide-and-Conquer Density-Functional Computational Method: Molecular Internal Rotation", The North Carolina Supercomputing Center, 1991.
4. Oral Contributed Presentation, "Direct Calculation of Electron Density: A Divide-and-Conquer Approach to Large Molecules", Fall meeting of the Southeastern Section of the American Physical Society, 1991.
5. Poster Presentation, "A Divide-and-Conquer Approach to Large Molecular and Solid-State Systems", 11th Canadian Symposium on Theoretical Chemistry, Montreal, Canada, 1992.
6. Oral Presentation, "Density Functional Approach to Large Molecules", 34th Congress of the International Union of Pure and Applied Chemistry, Beijing, China, 1993.
7. Poster Presentation, "Theory and Applications of a Divide-and-Conquer Method for Large Molecules", the 8th International Congress of Quantum Chemistry, Prague, Czech, July 19-23, 1994.
8. Poster Presentation, "Free energy calculations on enzyme reactions with an efficient iterative procedure to determine minimum energy paths on a combined ab initio QM/MM potential energy surface; Application to Enolase A Pseudo-Bond Approach To Combining Quantum Mechanical And Molecular Mechanical Methods ", the 10th International Congress of Quantum Chemistry, Menton, France, June 5-10, 2000.
9. Poster Presentation, "Nonorthogonal Localized Molecular Orbitals in Electronic Structure Theory ", Satellite Symposium of the 10th International Congress of Quantum Chemistry, Menton, France, June 11-14, 2000.

10. Invited Talk, (given by Postdoctoral Associate Haiyan Liu) "Quantum Mechanical Studies of Proteins: Enzyme Catalysis and Dynamics", Third International Workshop on Methods for Macromolecular Modeling, October 12-14, 2000.
11. Poster Presentation, (given by Postdoctoral Associate Yingkai Zhang) "Development of a DFT QM/MM free energy method for enzyme reactions", Third International Workshop on Methods for Macromolecular Modeling, October 12-14, 2000.
12. Poster Presentation, "Development of a DFT QM/MM free energy method for enzyme reactions and application to enolase", "We can do that" Symposium in Memory of Michael C. Zerner, Gainesville, Florida, November 16 - 18, 2000.
13. Poster Presentation, "Development of a DFT QM/MM free energy method for enzyme reactions and application to enolase", Sanibel Symposium, St. Augustine, Florida, February 24-March 2, 2001.
14. Poster Presentation, "Molecular Quantum Mechanics: The Right Answer for the Right Reason- An International Conference in Honor of Professor Ernest R. Davidson", Seattle, WA, July 22-26, 2001.
15. Contributed Talk, "Interactions in Isolated Quantum Dots: A Density Functional Theory Study", Hong, Jiang, Harold Baranger, Weitao Yang, American Physical Society March Meeting, Indianapolis, March 18-22, 2002.
16. Poster Presentation, Zhenyu Lu, Haiyan Liu, Weitao Yang, "A QM/MM Study on the Phosphodiesterase-Free Enzyme and Complex", American Chemical Society National Meeting, Orlando, April 7-11, 2002.
17. Poster Presentation, G. Andres Cisneros, Haiyan Liu, Yingkai Zhang and Weitao Yang, "QM/MM Study of the Reaction Mechanism of 4-Oxalocrotonate Tautomerase", American Chemical Society National Meeting, Orlando, April 7-11, 2002.
18. Poster, "Density Functional Theory Calculations with Correct Long Range Potentials", Qin Wu and Weitao Yang, Sandia National Laboratory Workshop on Quantum Mechanical Techniques: Exchange-Correlation Functional in Density Functional Theory, Albuquerque, New Mexico, August 14-16 2002
19. Invited Talk, "Coherence and Correlation in Electronic Nanostructures", Harold U. Baranger, Shailesh Chandrasekharan, and Weitao Yang, NSF Nanoscale Science and Technology Grantee Conference, December, National Science Foundation, Arlington, 11-13, 2002.
20. Contributed Talk, "Spin and Conductance Peak-Spacing Distributions in Isolated and Realistic Quantum Dots: A Density Functional Theory Study", Hong Jiang, H. U. Baranger, D. Ullmo and Weitao. Yang, American Physical Society Meeting, Austin, Texas, March, 2003.
21. Contributed Talk, "Addition Energy of Fullerenes and Carbon Nanotubes as Quantum Dots", San-Huang Ke, Harold U. Baranger, Weitao Yang, American Physical Society Meeting, Austin, Texas, March, 2003.
22. Poster, "Density Functional Theory Calculations with Correct Long Range Potentials", Qin Wu and Weitao Yang, the 225th ACS National Meeting (Division of Physical Chemistry), New Orleans, LA, March 23-27, 2003.

23. Poster, "Density Functional Theory Calculations with Correct Long Range Potentials", Qin Wu and Weitao Yang, the 225th ACS National Meeting (Division of Physical Chemistry), New Orleans, LA, March 23-27, 2003.
24. Poster, "OMP Decarboxylase: A Theoretical Investigation", Amy J. Boone, Jan Hermans, and Weitao Yang, Sanibel Symposium, St. Augustine, Florida, February 28 - March 5, 2004
25. Poster, "Minimum Energy Reaction Paths with The Method of Multipliers", Steven K. Burger and Weitao Yang, Sanibel Symposium, St. Augustine, Florida, February 28 - March 5, 2004
26. Poster, "Reaction Path Potential Derived from ab initio QM/MM Calculations", Zhenyu Lu, Minliang Wang and Weitao Yang, Sanibel Symposium, St. Augustine, Florida, February 28 - March 5, 2004
27. Poster, "A new second order perturbation theory energy functional within density functional theory", Paula Mori-Sanchez, Qin Wu, and Weitao Yang, Sanibel Symposium, St. Augustine, Florida, February 28 - March 5, 2004
28. Poster, "A direct optimization method for calculating density functionals and exchange correlation potentials from electron densities", Weitao Yang and Qin Wu, Sanibel Symposium, St. Augustine, Florida, February 28 - March 5, 2004
29. Poster, "A new second order perturbation theory energy functional within density functional theory", Paula Mori-Sanchez, Qin Wu, and Weitao Yang, Sanibel Symposium, St. Augustine, Florida, February 28 - March 5, 2004
30. Poster, "Algebraic equation and iterative optimization for the optimized effective potential in density functional theory", Qin Wu, and Weitao Yang, Sanibel Symposium, St. Augustine, Florida, February 28 - March 5, 2004
31. Poster, "The protein backbone makes important contributions to 4-oxalocrotonate tautomerase enzyme catalysis: Understanding from theory and experiment", G. Andres Cisneros, Peter Silinski, Michael C. Fitzgerald and Weitao Yang, Sanibel Symposium, St. Augustine, Florida, February 28 - March 5, 2004
32. Poster, "Transmission coefficient and free energy calculation for proton transfer in TIM on *Ab initio* QM/MM potential energy surface", Mingliang Wang, Zhenyu Lu and Weitao Yang, Sanibel Symposium, St. Augustine, Florida, February 28 - March 5, 2004
33. Contributed Talk, "Intermolecular Transport in Molecular Electronics Devices", Rui Liu, San-Huang Ke, H. Baranger, and Weitao Yang, American Physical Society Meeting, Montreal, Canada, March, 2004
34. Contributed Talk "Molecular Conductance: Effects of Contact Atomic Structure and Anchoring Group", San-Huang Ke, H. U. Baranger, and Weitao Yang, American Physical Society Meeting, Montreal, Canada, March, 2004
35. Contributed Talk, "Electron Transport Through Molecules: Self-consistent and Non-self-consistent Approaches", San-Huang Ke, H. U. Baranger, and Weitao Yang, American Physical Society Meeting, Montreal, Canada, March, 2004
36. Contributed Talk, "Gate and Scrambling Effects in Realistic Quantum Dots", Hong Jiang, D. Ullmo, H. U. Baranger, and Weitao Yang, American Physical Society Meeting, Montreal, Canada, March, 2004

37. Contributed Talk, "Spin Density Functional Calculations for Quantum Dots: How Much Can We Trust Them?" *Denis Ullmo*, Hong Jiang, Weitao Yang, and H. U. Baranger, American Physical Society Meeting, Montreal, Canada, March, 2004
38. Contributed Talk, "Quadratic String Method for determining the minimum energy path based on multiobjective optimization", *Steven Knox Burger* and Weitao Yang, symposium - "General Oral: Quantum Chemistry", The 232nd ACS National Meeting, San Francisco, CA, September 10-14, 2006
39. Contributed Talk, "Quadratic string method for determining the conformational change pathway of tryptophanyl-tRNA synthetase", *Steven Knox Burger*, Hao Hu and Weitao Yang, Symposium - "General Oral: Quantum Chemistry", The 232nd ACS National Meeting, San Francisco, CA, September 10-14, 2006
40. Poster, "Density Functional Theory Calculations with Correct Long Range Potentials", *Qin Wu* and Weitao Yang, the 225th ACS National Meeting (Division of Physical Chemistry), New Orleans, LA, March 23-27, 2003
41. Contributed Talk, "Reaction path potential for simulation of chemical reactions in enzymes derived from ab initio QM/MM calculations" Computational Chemical Dynamics in Honor of Don Truhlar, Minneapolis, October 7 -9, 2004
42. Contributed Talk, "Electron Transport Through Molecules: Gate Induced Polarization and Potential Shift", *SanHuang Ke*, H. U. Baranger, and Weitao Yang, American Physical Society Meeting, Los Angeles, March, 2005
43. Contributed Talk, "Organometallic Spintronics: Dicobaltocene Switch", *Rui Liu*, SanHuang Ke, H. U. Baranger and Weitao Yang, American Physical Society Meeting, Los Angeles, March, 2005
44. Contributed Talk, "Near-Perfect Conduction through a Single Molecular Orbital in a Ferrocene-Based Molecular Wire", *Michael S. Fuhrer*, Stephanie A. Getty, Chaiwat Engtrakul, Lixin Wang, Lawrence R. Sita, Rui Liu, San-Huang Ke, Harold U. Baranger and Weitao Yang, American Physical Society Meeting, Los Angeles, March, 2005
45. Poster, *Aron J. Cohen*, Paula Mori-Sanchez, and Weitao Yang, "Performance of the MCY functionals", Fifth Congress of the International Society for Theoretical Chemical Physics, New Orleans, Louisiana, July 20-26, 2005
46. Contributed Talk, "Potential Functionals: Theory and Application of the Optimized Effective Potential in Density Functional Theory", Weitao Yang, Pacificchem 2005, Honolulu, Hawaii, December 15-20, 2005
47. Contributed Talk, "Simulation of Biological Systems with Linear-Scale and Multi-Scale Approaches", Weitao Yang, Pacificchem 2005, Honolulu, Hawaii, December 15-20, 2005
48. Poster, *Paula Mori-Sanchez*, Aron J. Cohen and Weitao Yang, "Development of exchange-correlation functionals from the adiabatic connection", the XIIth International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006
49. Poster, *Aron Cohen*, Paula Mori-Sanchez and Weitao Yang, "Assessment of exchange correlation functionals from the adiabatic connection", the XIIth International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006

Dissertations Supervised

Tianhai Zhu (Ph. D) 1996

Dissertation title: Development and Application of Density Functional Methods for Electronic Structure Calculations of Solid-State Systems and Hydrogen-Bonded Systems.

Haihong Ni (MS) 1995

Thesis Title: Density Functional Study of Group III-V(13-15) Four-Membered Ring Compounds.

Taisung Lee (Ph. D.) 1997

Dissertation title: Linear -Scaling Quantum Calculations for Macromolecules.

Yingkai Zhang (Ph. D), 2000

Dissertation title: Development and Application of the Combined Quantum Mechanical/Molecular Mechanical Method and Density Functional Theory.

Qin Wu (Ph. D), 2004

Dissertation title: Improvement of the Exchange-Correlation Functional in Density Functional Theory.

Andreas Cisneros (Ph. D), 2004

Dissertation title: QM/MM Computational Studies and Theoretical Development: The Reaction Mechanism of 4-Oxalocrotonate Tautomerase.

Zhenyu Lu (Ph. D), 2005

Dissertation title: Computational Studies on Complex Systems: Theoretical Development and Applications

Rui Liu (Ph. D), 2006

Electronic Transport in Molecular Junctions

Current Group Members

Research Faculty

San-Huan Ke, Research Assistant Professor

Graduate Students

Steven Burger (Ph. D.)

Jerry Parks (Ph. D.)

Tim Heaton-Burgess (Ph.D.)

Fex Zeng (Ph.D.)

Postdocs

Bin Li

Felipe Bulat

Paula Mori-Sanchez

Aron Cohen

Hao Hu

Shahar Keinan

Xiangqiang Hu

Juan Qiao

Visiting Professors

Ruixue Xu (Univ. Sci. Tech. of China)

Mel Levy (North Carolina A & T)

Past Research Students/Postdocs

Undergraduate Students

	Period of Affiliation	Present Position
T. Daniel Crawford	1/91-5/92	Professor, V. Tech
Porter Mason	1/98-99	
Jason Donald		NSF Graduate Fellow, Harvard

Graduate Students

	Period of Affiliation	Present Position
Tianhai Zhu (Ph.D.)	12/91-4/96	Scientist, Accelrys Inc
Taisung Lee (Ph.D.)	12/92-3/97	senior Research Scientist, Univ. of Minnesota
Haihong Ni (MS)	12/93-5/95	NIH Postdoc Fellow at UC San Diego
Yingkai Zhang (Ph.D.)	12/96-5/00	Assistant Professor at New York University
Gerardo Andres Cisneros (Ph.D.)	12/00-6/04	Postdoc Fellow at NIEHS
Qin Wu (Ph.D.)	12/00-8/04	Postdoc Fellow at MIT
Zhenyu Lu (Ph.D.)	12/00-5/05	Postdoc Fellow at NYU
Rui Liu (Ph. D.)	12/01-5/06	

Postdocs

	Period of Affiliation	Present Position
Wei-Xiong Wu	11/89-11/90	Postdoc at NC State Univ.
Chengteh Lee	7/91-1/92	Manager/Scientist at AcuStaf Corporation
Surya Panigrahy	3/92-7/93	
Zhongxiang Zhou	4/91-12/91	Scientist at Alanex Corporation
Qingsheng Zhao	3/94-11/94	Scientist at AT and T
Jose Perez-Jorda	1/95-9/96	Associate Professor at University of Alicante, Spain
James Lewis	6/96-5/98	Assistant Prof. of Physics, Brigham Young Univ.
Yingkai Zhang	5/00-11/00	Assistant Professor at New York Univ.
Shubin Liu		Staff Scientist at the UNC, Chapel Hill
Haiyan Liu	11/98-11/00	Professor, University of Science and Technology, China
Darrin York (NSF fellow)	8/93-4/96	Assistant Professor at University of Minnesota
David Mazziotti (NSF fellow)		Assistant Professor at University of Chicago

Paul W. Ayers (NIH fellow)	06/01-07/02	Assistant Professor at University of MacMaster
Mingliang Wang	7/03-05/05	Assistant Prof. of Chemistry, Shenzheng Univ.
Takumi Hori	3/04-3/06	Researcher, Nippon Steel Chemical Co., Ltd.

Swedish Natural Science Research Council Postdoctoral Fellow

	Period of Affiliation	Present Position
Christer Enkvist	1/97-12/97	Uppsala University

Visitors/Visiting Professors

	Period of Affiliation	Present Position
Wei Pan	2/94-8/97	Graduate Student at Concordia University
Nicolas Cordero	Summer 3 months 95-97	Assistant Professor, Spain
Juvencio Robles	Summer 1996, 1998	Professor, Universidad de Guanajuato, Mexico
Jose Perez-Jorda	9/98-12/98	Associate Professor at University of Alicante, Spain
Hong Jiang (Ph. D.)	Visiting Graduate Student	Postdoc Fellow at Duke University
Robert Macglagan	Fall 2004	Professor, Univeristy of Canterbury
Chin-hui Yu	Fall 05-Spring 06	Professor, National Tsing Hua University

Teaching

Chem 161L

PHYSICAL CHEMISTRY LABORATORY (Fall 1991, Spring 1999)

Chem 161

PHYSICAL CHEMISTRY (Fall 1992, shared with Dr. P. Smith, Fall 1993, 1994, 1995, shared with Dr. D. B. Chesnut, Fall 1997, shared with Dr. A. T. McPhail)

Chem 161

ELEMENTS OF PHYSICAL CHEMISTRY (Fall, 2004)

Chem 203.1

INTRODUCTION TO QUANTUM MECHANICS I (Fall 1998, Fall 1999)

Chem 203.2

INTRODUCTION TO QUANTUM MECHANICS II (Fall 1998, Fall 1999)

Chem 207.2

THERMODYNAMICS (Fall 1989, 1990, 1991)

Chem 300

STATISTICAL MECHANICS (Spring 1992, 1993, 1994, 1995, 1996, shared with R.A. MacPhail Spring 1998, Spring 1999, Spring 2000)

Chem 302

QUANTUM MECHANICS (Spring 2000)

Chem 341

QUANTUM MECHANICS (Spring 2001, 2002)

Chem 303

SPECIAL TOPICS IN PHYSICAL CHEMISTRY (Spring 1992)

Chem 373

INDEPENDENT STUDY (Spring 1991, Fall 1991, Spring 1993, Spring 1998, Fall 1998, Spring 1999, Fall 2000)

Chem 377

RESEARCH ORIENTATION SEMINAR (Fall 1993)

MBP 292

ADVANCED PHYSICAL BIOCHEMISTRY: Tutorial Topics in Molecular Biophysics (Fall 2001)

Chem 342

QUANTUM MECHANICS (Spring 2003,2004)

CPS 258

INTRODUCTION TO COMPUTATIONAL SCIENCE (Fall 2003)

CPS 258L

INTRODUCTION TO COMPUTATIONAL SCIENCE LABORATORY (Fall 2003)

Review Service to Granting Agencies

National Science Foundation
Petroleum Research Fund
Research Corporation
Department of Energy
National Institute of Health

Review Service to Professional Journals

Canadian Journal of Chemistry
Chemical Physics Letters
International Journal of Quantum Chemistry
Journal of Chemical Physics
Journal of Physical Chemistry
Journal of Computational Physics
Physical Review A
Physical Review B
Physical Review Letters
Science
Theochem
International Journal of Quantum Chemistry
Theoretical Chemistry Account

University Service

1993:University Computational Task Force Subcommittee

2000-2001: Vice Provost John Harer's Advisory Committee on High Performance Supercomputing

2000-2001: Search Committee for the Director of Center for Computational Sciences and Engineering

2000-2002: Search Committee for the Director of Center of Bioinformatics and Computational Biology

2000-2003: Provost Advisory Committee on Appointment, Promotion and Tenure

2002-2003: Provost Task Force on Faculty Diversity

2002-2004: Arts and Science Computing Committee

2003-2005: Provost Standing Committee on Faculty Diversity

2004-2007: Provost Advisory Committee on Distinguished Professorship (Chair, 2006-07)

2004-2005: Search Committee for the Director of the Duke of Postdoctoral Services

2004-2005: Academic Council, alternate

2005-2007: Arts and Science Committee on Distinguished Professorship

Departmental Service

1989-1990: Computer Activity Committee
Graduate Recruiting Committee
Graduate Proficiency Exam Committee
Major Advising

1990-1991: Computer Activity Committee
Graduate Recruiting Committee
Graduate Proficiency Exam Committee
Major Advising

1991-1992: Seminar Committee (Chair)
Major Advising

1992-1993: Graduate Admission Committee
Seminar Committee

Major Advising

- 1993-1994: Graduate Admission Committee
Major Advising
- 1994-1995: Computer and Instrument Policy Committee
Graduate Curriculum Committee
Major Advising
- 1997-1998: Computer and Instrument Policy Committee (Chair)
Graduate Curriculum Committee
Major Advising
- 1998-1999: Computer and Instrument Policy Committee (Chair)
Personnel and Planning Committee
Major Advising
- 1999-2000: Computer and Instrument Policy Committee
Space Committee
Major Advising
Physical Chemistry Search Committee
Chair of the Theoretical Chemistry Search Committee
- 2000-2001: Computer and Instrument Policy Committee
Major Advising
Chair of the Theoretical Chemistry Search Committee
Faculty Review Committee
- 2001-2002: Faculty Review Committee
Space Committee
- 2002-2003: Faculty Review Committee
Chair of Space Committee
Ad Hoc Faculty Recruiting Committee
- 2003-2004: Chair of Space Committee
Ad Hoc Faculty Recruiting Committee

2004-2005: Secondary Appointment Committee

Tenure /Jr. Faculty Review Committee (Chair)

Crosscutting Inter-Departmental Opportunities Committee

Computer Committee (Chair)

Ad Hoc Search Committees

2005-2006: Senior Search Committee

Two Tenure and Promotion Committee

Proposition Exam Committee

Computer Committee