

# Weitao Yang

October 18, 2009

## 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

- 2010** 2010 International Solvay Chair in Chemistry, International Institutes for Physics and Chemistry, Brussels, Belgium.
- 2009** International Conference of Computational Methods in sciences and Engineering Prize for Distinguished Career in Computational Physics and Chemistry.
- 2006-present** Elected Member of the International Academy of Quantum Molecular Science, <http://www.IAQMS.org/>
- 2006** Humboldt Research Award for Senior U.S. Scientists.
- 2005-present** Recognized by the Institute for Scientific Information as a Highly Cited Researcher, <http://isihighlycited.com/>
- 1999-2006** 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 seven years from 1999 to 2006 since CAS started publishing citation data online: <http://www.cas.org/spotlight/bchem.html>. Number of Citations is over 25,000
- 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 Alfred P. 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, Advisory and Review Service

- International** Academic Advisory Committee, Hefei National Laboratory, China, 2007-2009
- NIH** Study Section: MSFD(Macromolecular Structure and Function) , November 2008,
- NIH** Study Section: MSFE(Macromolecular Structure and Function) , October 2007, October 2009
- NIH** Study Section: MSFD(Macromolecular Structure and Function) §Computational Biophysics" , October 2007

**NIH** Study section:Special Emphasis Panel/Scientific Review Group , July 2007  
**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  
**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

Elected Fellow of the American Association for the Advancement of Science  
Elected 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.

## References

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- [2] W. Yang, R. G. Parr, and R. Pucci, "Electron-density, kohn-sham frontier orbitals, and fukui functions," *Journal of Chemical Physics*, vol. 81, no. 6, pp. 2862–2863, 1984.
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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
106. Invited Talk, "Development in Density Functional Theory and Applications to Nanoscience", International Workshop on Computational Methods for Nanoscale Systems, Hong Kong, December 11-13, 2006
107. Invited Talk, "Accurate Density Functionals Addressing the Self-Interaction Error and Potential Functional Formalism", The Third International Workshop on DFT Applied to Metals and Alloys, Oran, Algeria, May 2-4 2007
108. Invited Talk, "Simulations of Complex Systems with Quantum Mechanics and Statistical Mechanics", Summer School, University of Science and Technology, Hefei, China, August 2-5, 2007
109. Invited Talk, "Free Energies of Chemical Reactions in Enzyme and in Solution" Symposium entitled "Quantum Mechanics and Statistical Mechanics: Can One Avoid the Other?", American Chemical Society National Meeting, Boston, August 19-23 2007
110. Invited Talk, "Accurate Density Functionals with Minimal Self-Interaction Error; Potential functional formalism", Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, American Chemical Society National Meeting, Boston, August 19-23 2007

111. Invited Talk, "Accurate Density Functionals with Minimal Self-Interaction Error; Potential functional formalism", DFT2007 Congress: Theory and Applications of DFT, Amsterdam, The Netherland, August 26-30, 2007
112. Invited Talk, "Linear Scaling Calculations with the Divide-and-Conquer Method and with Non-Orthogonal Localized Orbitals", 2007 Psi-k CECAM Workshop entitled "Linear-scaling ab initio Calculations: Applications and Future Directions", Lyon, France, September 3-6, 2007
113. Invited Talk, "Spin-Potential Functional Formalism for Current-Carrying Noncollinear Magnetic Systems", A Coastal Voyage of Current Density Functional Theory Tromsø - Trondheim, Norway, September 19-22, 2007
114. Invited Talk, "Simulation and Design of Complex Systems", Symposium on Photonics in the Translational Era: Science and Technology for a Purpose, Fitzpatrick Institute for Photonics Seventh Annual Meeting, Duke University, October 11-12, 2007
115. Invited Talk, "Fractional Number of Electrons: Insight and Progress in DFT", Gentner Symposium 2007: Time Dependent Density Functional Theory, Eilat, Israel, December 16-21, 2007
116. Invited Talk, "Theory and Simulation of Complex Systems: fractional charge, electron transport, and biocatalysis ", Mutiscale/Multiphysics Workshop, Office of Naval Research, Washington DC, February 5, 2008
117. Invited Talk, "Localization and Delocalization Error in DFT: from One-Electron Molecule to Bulk", Tulane DFT Fest: Honoring the Achievements of Prof. John P. Perdew, New Orleans, March 9, 2008
118. Invited Talk, "Fractional Charges and Fractional Spins in Density Functional Theory", Range Separated Hamiltonian Workshop, Paris, France, May 10-12, 2008
119. Invited Talk, "Free Energy of Chemical Reactions in Solution and in Enzymes with ab initio QM/MM-Minimum Free Energy Path method", the Wenner-Gren Foundations Lectures: Theoretical Biochemistry - Methods and Application, Stockholm, Sweden, May 14-17, 2008
120. Plenary Talk, "Fractional Charges and Fractional Spins in Density Functional Theory", The 10th National Conference on Quantum Chemistry, Nanjing, China, May 30-June 2, 2008
121. Invited Talk, "Free Energies of Chemical Reactions in Solution and in Enzymes with ab initio QM/MM Method", The 2008 Symposium on Computational Chemistry and HPC Applications, Qingdao, China, June 30 - July 3, 2008
122. Invited Talk, "Insights into Current Limitations of DFT", The Sixth Congress of the International Society for Theoretical Chemical Physics, Vancouver, Canada, July 19-24, 2008
123. Invited Talk, "Insights and Progress in Density Functional Theory", The World Association of Theoretical and Computational Chemists (WATOC) 2008, Sydney, Australia, September 14-19, 2008
124. Invited Plenary Talk, "Ab Initio QM/MM Minimum Free Energy Path for Chemical Reactions in Enzymes and in Solution", Theory and Applications of Computational Chemistry(TACC), an International Conference, Shanghai, China, September 23-27, 2008
125. Invited Talk, "Insights and Progress in Density Functional Theory from the Perspectives of Fractional Charges and Fractional Spins", Symposium on Density Functional Theory dedicated to Prof. José Luis Gázquez Mateos, Mexico City, Mexico, October 16-17, 2008
126. Invited Talk, "Overview: Free Energies of Chemical Reactions in Solution and in Enzymes with Ab Initio QM/MM", Workshop on Chemical Dynamics: Challenges and Approaches, Institute of Mathematics and Its Application, University of Minnesota, MN, January 12-16, 2009
127. Invited Talk, "Insight and Progress in Density Functional Theory: Perspectives of Fractional Charges and Fractional Spins", March Meeting of the American Physical Society, Pittsburgh, PA. March 16-20, 2009

128. Invited Talk, "Insights and Progress in Density Functional Theory", Spring Meeting of the German Physical Society, Dresden, Germany, March 24-27, 2009
129. Invited Talk, "Fractional charges and Fractional Spins", CORRELATED ELECTRONS IN MATTER, Sponsored Oak Ridge National Laboratory and Lawrence Livermore National Laboratory, Park Vista Hotel, Gatlinburg, Tennessee April 2-8, 2009
130. Plenary Lecture, "Developments in Density Functional Theory and ab initio QM/MM Methods for Catalysis", Department of Energy Basis Energy Catalysis Science Program Meeting, the Westin Hotel, Annapolis, MD, May 31-June 3, 2009
131. Invited Talk, "Insight and Progress in Density Functional Theory" ES09: 21th Annual Workshop on Recent Developments in Electronic Structure Methods, University of California, Davis, California, June 23-25, 2009
132. Invited Talk, "Free energies and mechanism of chemical reactions in solution and in enzymes with ab initio QM/MM method", CREST (Core Research for Evolutional Science and Technology) International Symposium on Theory and Simulations of Complex Molecular Systems, and International Symposium on Theory of Molecular Structure, Function and Reactivity, Celebrating Prof. Morokuma's 75th Birthday, Kyoto, Japan, July 19-21, 2009
133. Invited Talk, "Insight and Progress in Density Functional Theory", The Seventh Canadian Computational Chemistry Conference (CCCC7), Dalhousie University, Halifax, Nova Scotia, Canada, July 20-24, 2009
134. Plenary Talk, "Free energies and mechanisms of chemical reactions in enzymes and in solution with QM/MM minimum free energy path", Molecular Modelling (MM2009) Meeting, Mantra Legends Hotel, Gold Coast, Surfers Paradise, Queensland, Australia, July 26-29, 2009
135. Invited Talk, "Discontinuous nature of the exchange-correlation functional in strongly correlated systems", Symposium on New Developments in Strongly Correlated Electrons, ACS 238th National Meeting, Washington, DC. August 17, 2009
136. Invited Talk, "Free energies and mechanisms of chemical reactions in enzymes and in solution with QMMM minimum free energy path", Symposium on Protein Dynamics and Function, ACS 238th National Meeting, Washington, DC. August 17, 2009
137. Invited Talk, "Fractional charges and fractional spins: DFT to many-body theory", workshop on "Frontiers in Density functional Theory", Montauk, Long Island, New York, September 14-17, 2009
138. Invited Talk, "Insight and Progress in Density Functional Theory", Special Symposium in Honour of Professor Bernard Kirtman, International Conference on Computational Methods in Science and Engineering (ICCMSE), Hotel Rodos Palace, Rhodes, Greece, September 29- October 4 2009
139. Invited Talk, "Multiscale Modeling of Catalysis in Chemistry and Biology" Workshop on Theory and Applications of Multi-Scale Modeling, Duke University Center for Theoretical and Mathematical Scienc, September 11-12, 2009
140. Invited Talk, "Development and application of ab initio QM/MM methods for simulation of chemical reactions in solution and in enzymes", Symposium on Computational Quantum Chemistry, International Conference on Computational Methods in Science and Engineering (ICCMSE), Hotel Rodos Palace, Rhodes, Greece, September 29- October 4 2009

## 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 University, 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 Guanajuato, Mexico, May 3, 1999.

44. Invited Talk, "A Pseudo-Bond Approach To Combining Quantum Mechanical And Molecular Mechanical Methods", Department of Chemistry, University of Guanajuato, 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, "Nonorthogonal 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, "Computer 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.
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, Uptown, 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, 2006.
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
85. Invited Talk, Chemistry Seminar, "Conductance Through Single Molecules: What Molecules Can Do and How Well Theory Describes it", University of Michigan, Ann Arbor, September 28, 2006
86. Invited Talk, Seminar, "Going beyond B3LYP: Self-interaction-free exchange-correlation functionals for thermodynamics and kinetics", Sandia National Laboratory, Albuquerque, November 9, 2006
87. Invited Talk, Chemistry Seminar, "Simulations of Complex Biological Systems with Quantum Mechanics and Statistical Mechanics", University of New Mexico, Albuquerque, November 9, 2006
88. Invited Talk, Chemistry Seminar, "Simulations of Complex Biological Systems with Quantum Mechanics and Statistical Mechanics", Virginia Tech, Blacksburg, December 1, 2006
89. Invited Talk, Physics Seminar, "Designing Molecules and Materials by Optimizing Potentials", City University of Hong Kong, December 15, 2006
90. Invited Talk, Seminar, "Exploring enzyme function and drug design with the ab initio QM/MM approach", Roche Pharmaceuticals, Palo Alto, CA, March 14, 2007
91. Invited Talk, Pharmaceutical Sciences Seminar, "Simulations of Complex Biological Systems with Quantum Mechanics and Statistical Mechanics", College of Pharmacy, University of Kentucky, Lexington, Kentucky, May 11, 2007
92. Invited Talk, Computational Nanoscience Seminar, "Development in Density Functional Theory and Application to Electron Transport in Nanoscience", Cornell University, October 18, 2007
93. Invited Talk, Chemistry Colloquium, "Simulation of Complex Systems with Quantum and Statistical Mechanics", New York University, October 28, 2007
94. Invited Talk, Chemistry Colloquium Celebrating the Thirtieth Anniversary, "Simulation and Design of Complex Systems in Chemistry and Nanoscience", Universidad Autónoma Metropolitana, Mexico city, Mexico, November 6, 2007
95. Invited Talk, Physical Chemistry Seminar, "Fractional Number of Electrons: Insight and Progress in DFT for Chemistry and Nano-Material Science", University of California - Los Angeles, November 13, 2007
96. Invited Talk, Physical Chemistry Seminar, "Free Energy of Chemical Reactions in Solution and in Enzymes with Ab Initio QM/MM method", Wayne State University, Detroit, Michigan, April 30, 2008
97. Invited Talk, Physics Seminar, "Fractional Charges and Fractional Spins in Density Functional Theory", Tsinghua University, Beijing, China, May 28, 2008
98. Invited Talk, Chemistry Seminar, "Free Energy of Chemical Reactions in Solution and in Enzymes with Ab Initio QM/MM method", Beijing Normal University, Beijing, China, May 28, 2008
99. Invited Talk, Physics Seminar, "Conductance through Single Molecules", Anhui Normal University, Wuhu, China, July 5, 2008

100. Invited Talk, Chemistry Seminar, "Free Energy of Chemical Reactions in Solution and in Enzymes with Ab Initio QM/MM method", Nanjing University, Nanjing, China, July 8, 2008
101. Invited Talk, Seminar, "Free Energy of Chemical Reactions in Solution and in Enzymes with Ab Initio QM/MM method", Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China, July 10, 2008
102. Invited Talk, Physical Chemistry Seminar, "Free Energies and Mechanism of Chemical Reactions in Solution and in Enzymes with Ab Initio QM/MM Method", Department of Chemistry, University of North Carolina, Chapel Hill, November 3, 2008
103. Invited Talk, Physical Chemistry Seminar, "Free Energies and Mechanism of Chemical Reactions in Solution and in Enzymes with Ab Initio QM/MM Method", Department of Chemistry, University of North Carolina, Chapel Hill, November 3, 2008
104. Invited Talk, Physical Chemistry Seminar, "Free Energies and Mechanism of Chemical Reactions in Solution and in Enzymes with Ab Initio QM/MM Method", Department of Chemistry, California Institute of Technology, Pasadena, December 2, 2008
105. Invited Talk, "Free Energy Method for Enzymatic Reactions in Biological Systems and Its Implementation in a First-Principles QM/MM Package", Accelrys, San Diego, December 1, 2008
106. Invited Talk, "Free Energies and Mechanism of Chemical Reactions in Solution and in Enzymes with Ab Initio QM/MM Method", Chemistry Department Seminar, North Carolina State University, Raleigh, NC, February 6, 2009
107. Invited Talk, "Insights and Progress in Density Functional Theory-The Perspectives of Fractional Charge and Fractional Spin", Physics Department Colloquium, University of North Carolina, Chapel Hill, NC, April 27, 2009
108. Invited Talk, "Insights and Progress in Density Functional Theory-The Perspectives of Fractional Charge and Fractional Spin", Physics Department Colloquium, Virginia Commonwealth University, Richmond, VA, May 1, 2009
109. Invited Talk, "Insights and Progress in Density Functional Theory-The Perspectives of Fractional Charge and Fractional Spin", Physics Department Colloquium, University of Queensland, Australia, July 31, 2009
110. Invited Talk, "Free energies and mechanisms of chemical reactions in enzymes and in solution with QM/MM minimum free energy path", Physical Chemistry Seminar, University of Illinois, Urbana-Champaign, September 9, 2009