John Z.H. Zhang

1. Contact Address

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2. Education and Professional Experience

1978-1982	East China Normal University, B.S. in Physics
1982-1987	University of Houston, Ph. D in Chemical Physics
1987-1990	Research Associate, Department of Chemistry, UC Berkeley
1990-1994	Assistant Professor, Dept. of Chemistry, New York University
1994-1997	Associate Professor, Dept. of Chemistry, New York University
1997-	Professor, Dept. of Chemistry, New York University
1997	Visiting Professor, Hong Kong University of Science & Technology
2001	Visiting Professor, National University of Singapore
2001-2008	Founding Director, Institute of Theoretical & Computational Chemistry, Nanjing University
2005	Visiting Professor, Institute of Atomic and Molecular Science, Taiwan
2009-	Professor of Physics, East China Normal University
2013-	Professor of Chemistry, NYU Shanghai
2013-	Director, NYU-ECNU Center for Computational Chemistry, NYU Shanghai

3. Professional Service

Journal Editorship

1998-2002	*Theoretical Chemistry Accounts*, Advisor editor
2001-2008	*Journal of Theoretical and Computational Chemistry*, Editor-in-Chief
2008-	*Journal of Theoretical and Computational Chemistry*, Advisory editor
2002-	*Chinese Journal of Chemical Physics*, Editorial board
2008-12	*Science in China B-Chemistry*, Editorial board
2015-	*Scientific Reports*, Editorial board
2015-	*Chemical Physics Letters*, Editor
2015-	*Interdisciplinary Sciences: Computational Life Sciences*, Editorial board
2018-	*Molecular Based Mathematical Biology*, Editorial board

Professional Society

2011-	Member, Theoretical & Computational Chemistry Committee, Chinese Chemical Society
2010-2018	Member, Chemical Dynamics Committee, Chinese Chemical Society

2010-	Member, Protein Society Committee, Chinese Biochemistry and Molecular Biology Society
2010-	Member, Academic Committee, State Key National Lab of Chemical Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Science
2010-2017	Member, Academic Committee, Key Lab of Computational Material Science of MOE, Fudan University
2013-	Standing Committee Member, Shanghai Biophysical Society

4. Awards/Fellowships

1990 Camille and Henry Dreyfus New Faculty Award
1994 National Science Foundation Presidential Faculty Fellow
1995 Camille Dreyfus Teacher-Scholar
1995 Alfred P. Sloan Research Fellow
1999 Overseas Assessor of Chinese Academy of Science (中科院首批海外评审专家)
2000 Outstanding Overseas Young Investigator of NSFC (基金委海外杰出青年基金)

5. Major Research Accomplishment

1) Developed algebraic approach and successfully solved quantum reactive scatting problem for three-dimensional triatomic reactions.
2) Developed time-dependent wavepacket approach and successfully solved quantum reaction dynamics problem for (full) six dimensional tetratomic reactions.
3) Developed Molecular Fractional with Conjugate Caps (MFCC) approach for highly efficient linear scaling quantum chemical calculation of large complex molecular systems.
4) Developed protein-specific polarized charge (PPC) method for protein dynamics simulation with polarization effect.

6. Current Research Interest

Develop novel computational methods for accurate and efficient study of biological systems. Develop quantum and classical methods, including new polarized force field, to accurately predict protein structure, free energy in protein-drug and protein-protein bindings, conformational dynamics of membrane proteins, structure and dynamics of metalloproteins, drug design, etc.

7. Citations of Publications

Number of Publications: ~350
Number of times cited: >10,000
h-index: 52

8. Books

1. ***Dynamics of Molecules and Chemical Reaction***, edited by R. E. Wyatt and John Zeng Hui Zhang, (Marcel Dekker, New York, 1996).

2. ***Theory and Application of Quantum Molecular Dynamics***, John Zeng Hui Zhang, (World Scientific Publishing, Singapore, 1999).

9. Patent

1. Dawei Zhang and John Zeng Hui Zhang, "A METHOD FOR INTRODUCING CONJUGATED CAPS ONTO MOLECULAR FRAGMENTS AND SYSTEMS AND METHODS FOR USING THE SAME TO DETERMINE INTER-MOLECULAR INTERACTION ENERGIES", Patent No.: US 7,729,867 B2, Date of Patent: Jun. 1, 2010.

2. LEEHUANG S; LIN H P; ZHANG D; ZHANG J Z H; CHANG Y T; LEE J W; BAO J; SUN Y; HUANG P L, "Modulating adipocyte differentiation or adipogenic gene or lipolytic gene e.g. peroxisome proliferator activation receptor or their product expression used e.g. to treat obesity includes administering e.g. oleuropein and olive leave extract", US 2014296141A1; ; US9132145-B2, Nov. 5, 2013.

3. Lee-Huang, Sylvia; Huang, Paul L.; Huang, Philip Lin; Zhang, Dawei; Zhang, John Z. H.; Chang, Young Tae; Lee, Jae Wook; Bao, Ju; Sun, Yongtao, "Compositions and methods for treating obesity, obesity related disorders and for inhibiting the infectivity of human immunodeficiency virus", US 08574635

4. "一种非核苷类HIV-1反转录酶抑制剂", 专利号201310242563.7，Sept. 1, 2015

10. Invited Lectures at National/International Conferences

1. "S-matrix Kohn Variational Method for Quantum Reactive Scattering," Physics Computing '91, San Jose, California, July, 1991.

2. "Accurate Quantum Dynamics Studies Beyond Atom-Diatom Systems," Symposium on Chemical Dynamics in the Gas Phase, 207th ACS National Meeting, San Diego, California, March 13-17, 1994.

3. "Time-dependent Treatment for Diatom-Diatom Reactions," Symposium on Reactive Scattering, April APS National Meeting, Crystal City, VA, April 18-22, 1994.

4. "A full-dimensional time-dependent treatment for diatom-diatom reactions," Workshop on Quantum Mechanical Treatment of Atom Exchange Processes in Molecular Collisions, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, June 30-July 2, 1994

5. "Time-dependent Quantum Dynamics Studies for Chemical Reactions," Symposium on Computational Advances in Chemical Dynamics, 208th ACS National Meeting, Washington, DC, August 21-26, 1994.

6. "Time-dependent Treatment for Diatom-Diatom Reactions," The Fifth National Chemical Dynamics Conference, Jinan, Shandong, China, September 19-22, 1994.

7. "Time-dependent Quantum Dynamics Studies for Chemical Reactions," International Symposium on Computational Molecular Dynamics, University of Minnesota Supercomputer Institute, Minneapolis, MN, October 24-26, 1994.

8. "Steric Effect in Gas-phase and Gas-surface Reactions," Dynamics Workshop, Chester, United Kingdom, May 21-23, 1995.

9. "Time-dependent Approach to Quantum Reaction Dynamics," Conference on Molecular Energy Transfer (COMET) XIV, Kloster Banz, Germany, June 25–30, 1995.

10. "Time-dependent Approach to Chemical Dynamics Studies," Conference on the Dynamics of Molecular Collisions, Asiloma, CA, July 16–21, 1995.

11. "Quantum Dynamics of Chemical Reactions," The First Conference for Worldwide Young Chinese Chemists, Beijing, China, August 20–24, 1995.

12. "Dynamics studies of elementary chemical reactions," CCP6Workshop on Reaction Dynamics, Nottingham, England, August 30 – September 1, 1995.

13. "An overview of the time-dependent method in reactive scattering," 1996 Joint APS and AAPT meeting, Indianapolis, IN, 2-5 May, 1996.

14. "Accurate Polyatomic Quantum Dynamics Studies of Combustion Reactions," Eighteenth Combustion Research Conference, Tahoe City, CA, May 28-31, 1996.

15. Session Chair on "State-to-State Dynamics", Gordon Research Conference on Atomic and Molecular Interactions, Colby-Sawyer College, New London, NH, June 30-July 6, 1996.

16. "A new approach to state-to-state quantum reaction dynamics", Sanibel Conference, St. Augustine, Fl, March 1–7, 1997.

17. "A Reactant-Product Decoupling Approach to State-to-State Reaction Dynamic", Symposium on Interactions of Oriented Molecules, Bielefeld, Germany, June 30 –July 3, 1997.

18. "A Reactant-Product Decoupling Approach to State-to-State Polyatomic Reaction Dynamics." Worshop on Quantum Reactive Scattering, Telluride, Colorado, July 28–August 1, 1997.

19. "Correction of potential energy surface using inverse perturbation via singular value decomposition," Fifth Chemical Congress of North America, Cancun, Quintana Roo, Mexico, November 11-15, 1997.

20. "Dissociative chemisorption on metal surface: stereodynamics, symmetry effect, and fluctuation barrier," LASER TECHNIQUES FOR STATE-SELECTED AND STATE-TO-STATE CHEMISTRY IV, San Jose January 29-31, 1998

21. "Rigorous quantum dynamics study of the H2 + CN $\rightarrow$ HCN + H reaction in full dimensions," ACS Symposium on The Chemistry of of Combustion Processes, Dallas, Texas, March 29 - April 3, 1998.

22. "Time-dependent Study of Resonance States," CCP6 WORKSHOP ON QUANTUM STATES OF MOLECULES AT DISSOCIATION, University College London, 28-30 June, 1998

23. "A Reactant-Product Decoupling Approach to State-to-State Dynamics Calculation for Biomolecular Reaction and Unimolecular Fragmentation," Faraday Discussion No: 110

on Chemical Reaction Theory, University of St. Andrews, UK, July 1-3, 1998.

24. "A Reactant-Product Decoupling Approach to State-to-State Dynamics Calculation, "Worldwide Chinese Molecular Reaction Dynamice Symposium, Dalian, China, August 28-31, 1998.

25. "New Development in Quantum Reactive Scattering", Reactive ScatteringWorkshop, Perugia, Italia, June 25-27, 1999.

26. "A Practical Quantum Dynamical Model for Polyatomic Reaction", American Conference on Theoretical Chemistry, Boulder, Colorado, June 27 - July 2, 1999.

27. "Time-Dependent Approaches to Large Systems", First European Conference of Computational Chemistry, Perugia, Italia, June 28 - July 4, 1999.

28. "The SVRT model for Quantum Polyatomic Reaction Dynamics", Conference on Dynamics of Molecular Collisions, Split Rock, Pennsylvania, July 18-23, 1999.

29. "Ab Initio SOFA Quantum Dynamics for Chemical Reaction", The International Symposium on Photo-Dynamics and Reaction Dynamics of Molecules, Okazaki, Japan, July 31 - August 2, 1999.

30. "The SVRT model for polyatom-surface reaction", The Third European Conference on Gas-Surface Dynamics, Leiden, Netherland, September 26–28, 1999.

31. "A Divide and Conquer Partitioning Scheme for Rearrangement Collision", ITAMP workshop on Fragmentation and Recombination in Novel 3- and 4-Body Systems", Cambridge, MA, November 4-6, 1999.

32. "The SVRT model for polyatomic reaction dynamics", Biannual Workshop on Chemical Reaction Dynamics, Institute of Atomic and Molecular Science, Taipei, Taiwan, January 17-20, 2000.

33. "Quantum dynamics for polyatomic reactions", DYNAM 2000–A Symposium on Chemical Dynamics at the dawn of new millennium, Arcachon, France, May 32–June 2, 2000.

34. "Quantum dynamics for polyatomic reactions", First International Chinese Workshop on theoretical and computational chemistry, Dalian, China, August 14-17, 2000 (co-organizer).

35. "SVRT model for polyatomic reaction dynamics", Chemical Dynamics Symposium in honor of Bill Miller's 60th Birthday, Berkeley, CA, March 28-31, 2001.

36. "SVRT model for polyatomic reaction dynamics", CCP6 Workshop on Time-Dependent Quantum Dynamics, Bristol, UK, April 9-12, 2001.

37. "A General Model for Studying Polyatomic Reaction Dynamics", International Workshop on Computational Science and Engineering", Singapore, July 2, 2001.

38. "Quantum Reaction Dynamics: Theory and Computation", International Symposium on Frontiers in Molecular Science 2002, Qingdao, China, July 14-18, 2002.

39. “Chemical Reaction Dynamics: Theory and Computation”, 8th National Conference of Quantum Chemistry, Changchun, China, July 16-19, 2002.

40. “Study of polyatomic reactions beyond tetratomic systems”, Quantum Reactive Scattering Workshop, San Lorenzo de El Escorial, Spain, June 20-23, 2003.

41. “The SVRT model for quantum dynamics computation of polyatomic reactions”, Multidimensional Quantum Reaction Dynamics 2003, Freie Universit¨at Berlin, July 17 - 18, 2003.

42. “Semirigid vibrating rotor target model for polyatomic reaction”, XIth International Congress of Quantum Chemistry 2003, University of Bonn, Germany, July 20 - 26, 2003.

43. “An efficient linear-scaling method for quantum computation of protein interaction and applications to protein-drug bind”, Second Frontier Symposium in Theoretical and computational Chemistry of Nanjing University, China, May 21-23, 2004.

44. “Quantum Dynamics of Polyatomic reactions”, DICP Symposium on Molecular Dynamics, Dalian, July 21-23, 2004.

45. “New linear scaling method for quantum computation of proteins”, Advanced Symposium on Theoretical and Computational Chemistry of Chinese Academy of Science, Dalian, China, August 15-19, 2004.

46. “New Quantum Chemical Approach for Protein Studies”, International Workshop on Theoretical and Computational Chemistry of Complex Systems in conjunction with the 3rd Chinese Theoretical and Computational Chemistry Conference, The Hong Kong University of Science & Technology, Hong Kong SAR, China, January 3-7, 2005.

47. . Symposium on “The Computational Chemistry and Parallel Software”, Chinese Academy of Science, Yingtai, China, May 22-25, 2005.

48. “Quantum calculation of polyatomic reactions and protein energy”, The 9th Chinese Quantum Chemistry Conference, October 8-12, 2005, Guilin, China.

49. “Quantum study of protein”, 1st Cross Strait Symposium of Theoretical Chemistry, Xiamen, China, June 21-25, 2006.

50. “Polyatomic reaction dynamics”, The Computational Chemistry and Parallel Software, (CASSCCPS), Zhangjiajie, China, July 10-12, 2006.

51. “Global dynamics vs transition state theory”, Mathematics in Chemistry, a CIM Workshop, Lisbon, Portugal, July 19-21, 2006.

52. “Quantum methods for protein calculation”, Sixth Canadian Computational Chemistry Conference, British Columbia at Vancouver, Canada, July 26-30, 2006.

53. “Quantum method for protein solvation”, 4th WCTCC, Kunming, China, August 6-10, 2006. (plenary speaker).

54. “Quantum method for protein solvation”, Dewar Symposium, ACS National meeting in

San Francisco, California, September 10-14, 2006.

55. "Global dynamics and transition state in polyatomic reactions", Second DICP Symposium on chemical reaction dynamics, Dalian, China, Oct. 13-15, 2006.

56. "Quantum calculation of protein solvation", Barry Honig's 65th Birthday Symposium: Biological Applications of Implicit-Solvent Models March 25-29, 233rd ACS National Meeting, Chicago, IL 56. "Quantum study of protein energy", Autust 10-12, WFTCP C-07, Qingdao, China,2007.

57. "Protein dynamics using polarized protein force field", Sept. 20-24, Dynamics of Molecular Collisions, Dalian, China, 2007.

58. "Quantum mechanical study of protein in solution", October 18-21, Third International Conference on Theoretical Chemistry, Molecular Modeling and Life Sciences, Yantai, China, 2007 (plenary speaker).

59. 2nd Cross-Strait Theoretical and Computational Chemistry Conference (CTCC-2), Academic Sinica, Taiwan, April 14-18, 2008.

60. 1st International Conference of the Grand Challenge to Next-Generation Integrated Nanoscience, "Development & Application of Advanced High-Performance Supercomputer" Project (MEXT), Tokyo, Japan, June 3 to 7, 2008.

61. CAS Symposium on Computational Chemistry and HPC Applications Qingdao, China, June 29—July 3, 2008.

62. 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, Canada, July 19-24, 2008 (plenary speaker).

63. 49th Sanibel Symposium, St. Simons, Georgia (invited speaker), Feb. 26- March 3, 2009.

64. Quantum Reactive Scattering (QRS) Workshop, Dalian, China, June 6-10, 2009.

65. Eleventh National Chemical Dynamics Conference of China, Yichang, Hubei, Aug. 13-17, 2009.

66. 238th ACS National Meeting, Washington, DC, USA, "The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry" Aug. 16-20, 2009.

67. Fourteenth International Workshop on Quantum Systems in Chemistry and Physics (QSCP-XIV), San Lorenzo del Escorial, Madrid, Spain, Sep. 13-19, 2009.

68. International Conference on Computational and System Biology (ICCSB), Shanghai, China, Oct. 9-11, 2009.

69. 2009 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry, Suzhou, China, Oct. 30-Nov. 2, 2009.

70. 5th Worldwide Chinese Theoretical and Computational Chemistry Conference (WCTCC), Xiamen, China, Dec. 14-17, 2009 (invited speaker)

71. 27th national meeting, Chinese Chemical Society, Xiamen, China, 2010, June 19-23, 2010 (invited speaker).

72. Symposium on Theoretical Study of Superamolecules, Jiling University, Jiling, China, July 2-3, 2010 (invited speaker).

73. fourth International Conference on Biophysics and Molecular Biology, Shanghai, China, Aug 8-12, 2010 (invited speaker).

74. The 4th Cross-Strait Theoretical and Computational Chemistry Conference (CTCC-4), Jinmeng, Taiwan, January 10-14, 2011 (invited speaker).

75. The 3dr APPA Conference in Conjunction with the 3rd Symposium of the CPS and, Joint Sino-UK Meeting, Shanghai University, China, May 5-9, 2011 (invited speaker).

76. The 11th National Conference of Quantum Chemistry, Heifei, China, May 27-30, 2011 (invited speaker).

77. The 12th National Chemical Dynamics Symposium, Chengdu, China, June 10-14, 2011 (invited speaker).

78. Physical Chemistry Summer School, Guangzhou, China, August 8-19, 2011 (lecturer).

79. International Conference on Theoretical and High Performance Computational Chemistry，ICT-HPCC11, Xi An, China, August 11-14, 2011 (invited speaker)

80. Symposium on frontier theoretical and computational chemistry, Dalian, China, August 16-19, 2011 (invited speaker).

81. 2011 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry, Haikou, China, December 21- 24, 2011 (co-organizer).

82. International Conference on Theoretical and High Performance Computational Chemistry, Nanjing, China, July 8-11, 2012 (invited speaker).

83. Physical Chemistry Summer School, South China Normal University, Guangzhou, China, August 6, 2012 (lecturer).

84. The 5th Cross-Strait Theoretical and Computational Chemistry Conference (CTCC-5)), Xi An, China, August 7-10, 2012 (invited speaker).

85. First World Wide Chinese Computational Biology and Molecular Simulation Conference, Dalian, China, August 10-13, 2012 (organizer).

86. 2012 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry, Hong Kong, China, December 1-3, 2012 (invited speaker).

87. "International Symposium of Theoretical and Computational Chemistry, Fudan University, Shanghai, China, March 22-24, 2013 (invited speaker).

88. "6th Worldwide Chinese Theoretical and Computational Chemistry Conference

(WCTCC), New Taipei City, Taiwan, June 24-28, 2013 (invited speaker).

89. "ACS meeting", Indianapolis, IN, Sept. 8-12, 2013 (invited speaker).

90. "4th Cross Disciplinary Symposium in Protein Research", Heifei, Anhui, China, Oct. 12-14, 2013 (invited speaker).

91. 2013 WFTCPC", Tide Resort, Thailand, Dec. 8-12, 2013 (co-organizer and invited speaker).

92. International Symposium in Theoretical and Computational Chemistry, East China University of Science & Technology, Shanghai, April 20-22, 2014 (invited speaker).

93. Computational Chemistry International Symposium, NYU-ECNU Center for Computational Chemistry, NYU Shanghai, May 23-25, 2014 (organizer)

94. The 12th National Conference on Quantum Chemistry, Taiyuan, China, June 12-15, 2014 (invited speaker).

95. International Symposium on Laser and Computational Biophysics, Shanghai, June 15-17, 2014 (organizer)

96. The 8th Joint Meeting of Chinese Physicists Worldwide (OCPA8), Singapore, June 23-27, 2014 (invited speaker).

97. The 3rd National Conference on Biophysical Chemistry, Qingdao, July 23-26, 2014 (invited speaker).

98. Annual ACS meeting in San Francisco, Computers in Chemistry, August 10-14, 2014 (invited speaker).

99. WFTCPC14, Quzhou, China, August 21-24, 2014 (invited speaker).

100. The Second International Workshop on Computational Science and Engineering, HONG KONG, Dec 12-16, 2014 (Coordinator and Plenary Speaker).

101. The sixth across strait Theoretical Chemistry Conference, Jiayi, Taiwan, Jan 26-30, 2015 (invited speaker).

102. Frontiers in Polymer and Biomolecular Chemistry Conference, TAU, Israel，March 2-4, 2015 (invited speaker).

103. Symposium on Dynamics of Complex Systems，University of Science and Technology, Heifei, Anhui, China, April 11, 2015 (invited speaker).

104. Strategic Symposium on Theoretical and Computational Chemistry, Liyang, Jiangsu, April 25-26, 2015 (invited speaker).

105. "Satellite meeting on simulations of macromolecular systems, in association with the 2015 ICQC", Changchun, Jilin, China, June 4-7, 2015 (invited speaker).

106. NYUSH International Symposium on Frontiers in Computational Chemistry, NYU Shanghai, August 23-26, 2015 (organizer).

107. Symposium on Multiple Faces of Biomolecular Electrostatics, Ohio State University, October 12-16, 2015 (invited speaker).

108. The Seventh Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC 7), Kaohsiung, Taiwan, January 25-28, 2016 (invited speaker).

109. IAS Focused Program on Molecular Machines of Life: Simulation Meets Experiment", HKUST, May 23-27, 2016 (invited speaker).

110. Sino-German Workshop n Biomolecular Simulations Across Scales, Shanghai, May 26-30, 2016 (invited speaker).

111. The fourth National Conference on Biophysical Chemistry, Heifei, June 14-17, (session chair)

112. 2016 Shanghai Frontier workshop in molecular biophysics, NYU Shanghai, July 22-25, 2016 (organizer).

113. International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry, Nanchang, China, August 13-16, 2016 (invited speaker).

114. 7th Cross-strait Theoretical and Computational Chemistry (CTCC-7) conference, Changsha, Hunan (speaker), Oct. 14-18, 2016 (invited speaker)

115. The 4th International Conference on Molecular Simulation, Shanghai, China, Oct. 23-26, 2016 (plenary speaker)

116. Shanghai-Stockholm Bilateral Conference on Theoretical Chemistry, Shanghai, China, Oct. 31-Nov. 3, 2016 (invited speaker).

117. ZIRI Spring Symposium 2017 at HKU Zhejiang Institute of Research and Innovation, Lin'an, Zhejiang, China, March 17, 2017 (plenary speaker).

118. The 6th Chinese-French Workshop in Theoretical Chemistry (CFWTC2017), Xiamen, China, May 7-10, 2017 (invited speaker).

119. 6/8-11, The 13th National Conference in Quantum Chemistry, Dalian, China, June 8-11, (invited speaker).

120. 6/12-16, IC3 Summer School, NYU Shanghai, China, June 12-16, 2017 (co-organizer)

121. Ultrafast Vibrational Spectroscopy Conference, Chinese Academy of Science, Beijing, China, July 17-19 (invited speaker).

122. OCPA9 conference, Tsinghua University, Beijing, China, July 17-20, 2017 (invited speaker)

123. International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry (WFTCPC17), Guiyang, China, August 3-6, 2017 (organizer & invited

speaker).

124. COMP Division's National ACS Meeting in Washington, DC, August 20-24, 2017 (invited speaker).

125. Chinese Protein Society Annual Conference, Guangzhou, China, September 21-24, 2017 (invited speaker).

126. International Conference on Theoretical and High Performance Computational Chemistry 2017 (ICT-HPCC17), Hangzhou, China, October 26-29, 2017 (invited speaker).

127. The 2nd Conference in Artificial Intelligence, Precision Biomedicine and Bioinformatics, Shanghai, China, December 20-21, 2017 (invited speaker).

List of Research Publications:

1. Z.H. Zhang, N. Abusalbi, M. Baer, D.J. Kouri, and J. Jellinek, "Resonance Phenomena in Quantal Reactive Infinite-Order Sudden Calculations," ACS Symposium Series 263, 457 (1984).

2. Z.H. Zhang, and D.J. Kouri, "A Wave Packet Solution to the Time-Dependent Arrangement Channel Quantum Mechanics Equations," Phys. Rev. A 34, 2687 (1986).

3. K. Haug, D.W. Schwenke, Y. Shima, D.G. Truhlar, J.Z.H. Zhang, and D.J. Kouri, "L2 Solution of the Quantum mechanical Reactive Scattering Problem. The Threshold Energy for D + H2(v=1) $\rightarrow$HD + H," J. Phys. Chem. 90, 6757 (1986).

4. Y.C. Zhang, Z.H. Zhang, and D.J. Kouri, "Infinite Order Sudden Approximation treatment of the H + D2 ! HD + D Reaction," Chem. Phys. 114, 267 (1987).

5. K. Haug, D.W. Schwenke, D.G. Truhlar, Y. Zhang, J.Z.H. Zhang, and D.J. Kouri, "Accurate Quantum Mechanical Reaction Probabilities for the reaction O + H2 → OH + H," J. Chem. Phys. 87, 1892 (1987).

6. J.Z.H. Zhang, Y. Zhang, D.J. Kouri, B.C. Garrett, K. Haug, D.W. Schwenke, and D.G. Truhlar, "L2 Calculations of Reactive Scattering Transition Probabilities," Faraday Disc. Chem. Soc. 84, 371 (1987).

7. D.W. Schwenke, K. Haug, D.G. Truhlar, Y. Sun, J.Z.H. Zhang, and D.J. Kouri, "Variational Basis- Set Calculations of Accurate Quantum Mechanical Reactive Probabilities," J. Phys. Chem. 91, 6080 (1987).

8. D.W. Schwenke, K. Haug, D.G. Truhlar, R.H. Schweitzer, J.Z.H. Zhang, Y. Sun, and D.J. Kouri, "Storage Management Strategies in Large-Scale Quantum Dynamics Calculations," Theor. Chem. Acta. 72, 237 (1987).

9. J.Z.H. Zhang and W.H. Miller, "New Method for Quantum Reactive Scattering, with Applications to the 3-D H + H2 Reaction, "Chem. Phys. Lett. 140, 329 (1987).

10. J.Z.H. Zhang, D.J. Kouri, K. Haug, D.W. Schwenke, Y. Shima, and D.G. Truhlar, "L2 Amplitude Density Method for Multichannel Inelastic and Rearrangement Collisions," J. Chem. Phys. 88, 2492 (1988).

11. Y. Zhang, J.Z.H. Zhang, D.J. Kouri, K. Haug, D.W. Schwenke, and D.G. Truhlar, "Quantum Mechanical Calculations of Vibrational Population Inversion in Chemical Reactions: Numerically Exact L2 Amplitude Density Study of the H2Br Reactive System," Phys. Rev. Lett. 60, 2367 (1988).

12. D.W. Schwenke, K. Haug, M. Zhao, D.G. Truhlar, Y. Sun, J.Z.H. Zhang, and D.J. Kouri, "Quantum Mechanical Algebraic Variational Methods for Inelastic and Reactive Molecular Collisions," J. Phys. Chem. 92, 3202, (1988).

13. J.Z.H. Zhang, S.I. Chu, and W.H. Miller, "Quantum Scattering via the S-Matrix Version of the Kohn Variational Principle," J. Chem. Phys. 88, 6233 (1988).

14. J.Z.H. Zhang and W.H. Miller, "Accurate 3-Dimensional Quantum Scattering Calculations for F + H2 →HF + H," J. Chem. Phys. 88, 4549 (1988).

15. J.Z.H. Zhang and W.H. Miller, "Quantum Reactive Scattering via the S-Matrix Version of the Kohn Variational Principle: Integral Cross Section for H + H2(v=j=0) → H2(v'=1,j'=1,3) + H in the Energy.Range Etot(eV)=0.9-1.4," Chem. Phys. Lett. 153, 465 (1988).

16. J.Z.H. Zhang andW.H. Miller, "Comment on: Quantum Reactive Scattering via the S-Matrix Version of the Kohn Variational Principle," J. Chem. Phys. 89, 4454 (1988).

17. D.J. Kouri, Y. Sun, R.C. Mowrey, J.Z.H. Zhang, D.G. Truhlar, K. Haug, and D.W. Schwenke, in Mathematical Frontiers in Computational Chemical Physics, edited by D.G. Truhlar (Springer, New York, 1988), p. 207.

18. J.Z.H. Zhang and W.H. Miller, "Quantum Reactive Scattering via the S-Matrix Version of the Kohn Variation Principle: Differential and Integral Cross Section for D + H2 → HD + H," J. Chem. Phys. 91, 1528 (1989).

19. J.Z.H. Zhang and W.H. Miller, "Differential Cross Section (Angular Distribution) for the Reaction H + H2(v=j=0) → H2(v',odd j') + H in the Energy Range 0.90 - 1.35 eV," Chem. Phys. Lett. 159, 130 (1989).

20. J.Z.H. Zhang, "Interaction Representation in Time Dependent Quantum Scattering: Elimination of Finite Boundary Reflection," Chem. Phys. Lett. 160, 417 (1989).

21. J.Z.H. Zhang, "New Method in Time Dependent Quantum Scattering Theory: Integrating the Wave Function in the Interaction Picture," J. Chem. Phys. 92, 324 (1990).

22. J.Z.H. Zhang andW.H. Miller, "Photodissociation and Continuum Resonance Raman Cross Sections, and general Franck-Condon intensities, from S-matrix Scattering Calculations, with applications to the photoelectron spectrum of $H2F^-$ → H2 + F, HF + H + e–", J. Chem. Phys. 92, 1811 (1990).

23. S.M. Auerbach, J.Z.H. Zhang andW.H. Miller, "Comparison of Quantum Scattering Calculations for the H + H2 Reaction Using the LSTH and DMBE Potentials", J. Chem. Soc.

Faraday Trans. 86, 1 (1990).

24. J.Z.H. Zhang and W.H. Miller, "Quasi-Adiabatic Basis Functions for the S-Matrix Kohn Variational Approach to Quantum Reactive Scattering", J. Phys. Chem. 94, 7785 (1990).

25. R.E. Continetti, J.Z.H. Zhang and W.H. Miller, "Comment on: Resonance structure in the energy dependence of state-to-state differential scattering cross sections for the D + H2(v,j) → HD(v',j') + H reaction", J. Chem. Phys. 93, 5356 (1990).

26. J.Z.H. Zhang, D.L. Yeager, and W.H. Miller, "3D Quantum Scattering Calculations of the Reaction He + H+2 → HeH+ + H for Total Angular Momentum J=0", Chem. Phys. Lett. 173, 480 (1990).

27. J.Z.H. Zhang, "Multichannel Quantum Wave Packet Propagation in the Interaction Picture: Application to Gas-Surface Scattering", Comput. Phys. Commun. 63 28 (1991).

28. W.H. Miller and J.Z.H. Zhang, "How to Observe the Elusive Resonances in H or D + H2 → H2 or HD + H Reactive Scattering", J. Phys. Chem. 95, 12 (1991).

29. J.Z.H. Zhang, "Progress of Basis Optimization Techniques in Variational Calculation of Quantum Reactive Scattering", J. Chem. Phys. 94, 6047 (1991).

30. J.Z.H. Zhang, "Variational Calculation of Integral Cross Sections for the Reaction F + H2 → HF + H", Chem. Phys. Lett. 181, 63 (1991).

31. J.Z.H. Zhang,W.H. Miller, AlexandraWeaver, and Daniel M. Neumark, "Quantum Reactive Scattering Calculations of Franck-Condon Factors for the Photodetachment of H2F− and D2F− and Comparisons with Experiment", Chem. Phys. Lett. 182, 283 (1991).

32. D.H. Zhang and J.Z.H. Zhang, "Time-dependent Treatment of Vibrational PredissociationWithin the Golden Rule Approximation", J. Chem. Phys. 95, 6449 (1991).

33. Z. Bacic and J.Z.H. Zhang, "A New D_{3h}Symmetry Adapted Method for Highly Excited Vibrational Levels of Floppy Triatomics: The H+3 Molecule", Chem. Phys. Lett. 184, 513 (1991).

34. D.H. Zhang and J.Z.H. Zhang, "An Efficient Time-dependent Golden Rule Treatment for Vibrational Predissociation of HeI2," J. Phys. Chem. 96, 1575 (1992).

35. Z. Bacic and J.Z.H. Zhang, "High-Lying Rovibrational States of Floppy X3 Triatomics by a New D3h Symmetry Adapted Method: Application of the H+3 Molecule", J. Chem. Phys. 96, 3707 (1992).

36. J.Z.H. Zhang, "A Stochastic Golden-Rule Treatment for Thermal Desorption of Gases from Solid Surfaces", J. Chem. Phys. 96, 4729 (1992).

37. J. Sheng and J.Z.H. Zhang, "Dissociative chemisorption of H2 on Ni surface: time-dependent quantum dynamics calculation and comparison with experiment," J. Chem. Phys. 96, 3866 (1992).

38. J. Sheng and J.Z.H. Zhang, "Theoretical model for the dynamics of hydrogen recombination

on Si(100)-(2×1) surface," J. Chem. Phys. 97, 596 (1992).

39. D.H. Zhang, J.Z.H. Zhang, and Z. Bacic, "A time-dependent golden rule wave packet calculation for vibrational predissociation of D2HF," J. Chem. Phys. 97, 927 (1992).

40. D.H. Zhang, J.Z.H. Zhang, and Z. Bacic, "Mode-specific decay widths in vibrational predissociation of D2HF," Chem. Phys. Lett. 194, 313 (1992).

41. D.H. Zhang, J.Z.H. Zhang, and Z. Bacic, "A time-dependent calculation for vibrational predissociation of H2HF," J. Chem. Phys. 97, 3149 (1992).

42. D.H. Zhang and J.Z.H. Zhang, "Vibrational predissociation in HD-HF," Chem. Phys. Lett. 199, 187 (1992).

43. D.H. Zhang, O.A. Sharafeddin, and J.Z.H. Zhang, "Product state distribution in time-dependent quantum wave packet calculation with an optical potential," Chem. Phys. 167, 137 (1992).

44. J. Sheng and J.Z.H. Zhang, "An algebraic variational approach to dissociative adsorption of a diatomic molecule on a smooth metal surface," J. Chem. Phys. 97, 6784 (1992).

45. J.Z.H. Zhang, "Quantum reactive scattering using the S-matrix Kohn variational method," Int. J. Mod. Phys. C3 1351 (1992).

46. Sharafeddin and J.Z.H. Zhang, "A DVR based time-dependent wave packet treatment for reactive scattering," Chem. Phys. Lett. 204, 190 (1993).

47. D.H. Zhang and J.Z.H. Zhang, "Total and partial decay widths in vibrational predissociation of HF dimer," J. Chem. Phys. 98, 5978 (1993).

48. D.H. Zhang and J.Z.H. Zhang, "Quantum mechanical calculation for photodissociation of hydrogen peroxide," J. Chem. Phys. 98, 6276 (1993).

49. J. Sheng and J.Z.H. Zhang, "Quantum dynamics studies of adsorption and desorption of hydrogen at a Cu (111) surface," J. Chem. Phys. 99, 1373 (1993).

50. D.H. Zhang and J.Z.H. Zhang, "Accurate quantum calculation for the benchmark reaction H2 + OH → H2O + H in five-dimensional space: Reaction probabilities for J=0," J. Chem. Phys. 99, 5615 (1993).

51. D.H. Zhang and J.Z.H. Zhang, "Photofragmentation of HF dimer: Quantum dynamics studies on ab initio potential energy surfaces," J. Chem. Phys. 99, 6624 (1993).

52. D.H. Zhang and J.Z.H. Zhang, "Accurate quantum calculations for H2 + OH → H2O + H: Reaction probabilities, cross sections, and rate constants," J. Chem. Phys. 100, 2697 (1994).

53. Z.T. Cai, D.H. Zhang, and J.Z.H. Zhang, "Quantum dynamical studies for photodissociation of H2O2 at 248 and 266 nm," J. Chem. Phys. 100, 5631 (1994).

54. D.H. Zhang and J.Z.H. Zhang, "A full-dimensional time-dependent treatment for diatom-diatom reactions: the H2 + OH reaction," J. Chem. Phys. 101, 1146 (1994).

55. J.Q. Dai, J. Sheng, and J.Z.H. Zhang, "Symmetry and rotational orientation effects in dissociative adsorption of diatomic molecules on metals: H2 and HD on Cu(111)," J. Chem. Phys. 101, 1555 (1994).

56. D.H. Zhang and J.Z.H. Zhang, "Quantum reactive scattering with a deep well: time-dependent calculation for H + O2 reaction and bound state characterization for HO2," J. Chem. Phys. 101, 3671 (1994).

57. J.Q. Dai and J.Z.H. Zhang, "Steric effect in dissociative chemisorption of hydrogen on Cu," Surf. Sci. 319, 193 (1994).

58. D.H. Zhang, Q. Wu, and J.Z.H. Zhang, "A time-dependent approach to flux calculation in molecular photofragmentation: vibrational predissociation of HF-DF," J. Chem. Phys. 102, 124 (1995).

59. D.H. Zhang and J.Z.H. Zhang, "Accurate time-dependent quantum scattering calculation for diatomdiatomreaction with branching: HD + OH → H + DOH, D + HOH," Chem. Phys. Lett. 232, 370 (1995).

60. D.H. Zhang, Q. Wu, J.Z.H. Zhang, M.v. Dirke, and Z. Bacic, "Exact full-dimensional bound statecalculations for (HF)2, (DF)2, and HFDF," J. Chem. Phys. 102, 2315 (1995).

61. M.v. Dirke, Z. Bacic, D.H. Zhang, and J.Z.H. Zhang, "Vibrational predissociation of HF dimer inv =1: influence of initially excited intermolecular vibrations on the fragmentation dynamics," J. Chem. Phys. 102, 4382 (1995).

62. J. Dai and J.Z.H. Zhang, "Quantum adsorption dynamics of a diatomic molecule on surface: 4- dimensional fixed-site model for H2 on Cu (111)," J. Chem. Phys. 102, 6280 (1995).

63. D.H. Zhang, J.Z.H. Zhang, Y.C. Zhang, D.Y. Wang, and Q.G. Zhang, "Quantum dynamics study of the reaction HD + OH! H + DOH, D + HOH," J. Chem. Phys. 102, 7400 (1995).

64. J. Dai and J.Z.H. Zhang, "Noise-free spectrum for time-dependent calculation of eigenenergies," J. Chem. Phys. 103, 1491 (1995).

65. Q. Wu, D.H. Zhang, and J.Z.H. Zhang, "6D quantum calculation of energy levels for HF stretching excited (HF)2," J. Chem. Phys. 103, 2548 (1995).

66. D.H. Zhang and J.Z.H. Zhang, "Quantum calculations of reaction probabilities for HO + CO → H +CO2 and bound states of HOCO," J. Chem. Phys. 103, 6512 (1995).

67. Y.C. Zhang, D.H. Zhang, W. Li, Q.G. Zhang, D.Y. Wang, D.H. Zhang, J.Z.H. Zhang, "Quantum dynamics study for D2 + OH reaction," J. Phys. Chem. 99, 16824 (1995).

68. Da-Ren Guan, Xian Zhao, Cong-Hao Deng, and John Z.H. Zhang, "Time-dependent golden rule wave packet treatment for vibrational predissociation of HeI2 molecule for low initial vibrational excitations," Jiegou Huaxue, 14, 384 (1995).

69. J. Dai and J.Z.H. Zhang, "Time-dependent spectral calculation of bound and resonance energies of HO2," J. Chem. Phys. 104, 3664 (1995).

70. T. Peng, D. H. Zhang, J. Z.H. Zhang, and R. Schinke "Reaction of O(1D) + H2 → HO +H, A three dimensional quantum dynamics study," Chem. Phys. Lett. 248, 37 (1996).

71. Q. Wu and J. Z.H. Zhang, "Correction of potential energy surface using inverse perturbation and singular value decomposition," Chem. Phys. Lett. 252, 195 (1996).

72. J. Dai and J.Z.H. Zhang, "Time-dependent wavepacket approach to state-to-state reactive scattering and application to H + O2 reaction," J. Phys. Chem. 100, 6898 (1996).

73. J.Y. Ge, J. Dai and J.Z.H. Zhang, "Dissociative adsorption of O2 on Cu(110) and Cu(100): three dimensional quantum dynamics studies," J. Phys. Chem. 100, 11432 (1996).

74. W. Yu and C.F. Wong, and J.Z.H. Zhang, "Brownian Dynamics Simulations of Polyalanine in Salt Solutions," J. Phys. Chem. 100, 15280 (1996).

75. W. Zhu, Jiqiong Dai, and John Z.H. Zhang, "State-to-state time-dependent quantum calculation for reaction H2 + OH! H + H2O in six dimensions," J. Chem. Phys. 105, 4881 (1996).

76. Jiqiong Dai, Wei Zhu, and John Z. H. Zhang, "Energy-dependence of state-to-state reaction probabilities for H2 + OH-> H + H2O in six dimensions," J. Phys. Chem. 100, 13901 (1996).

77. Zhang, D. H.; Zhang, J. Z.H., "Time-dependent Quantum Dynamics for Gas-Phase and Gas-Surface Reactions," in Dynamics of Molecules and Chemical Reactions, ed., R.E. Wyatt and J.Z.H. Zhang, (Marcel Dekker, New York, 1996), p. 231.

78. Tong Peng and John H. Z. Zhang, "A reactant-product decoupling method for state-to-state reactive scattering," J. Chem. Phys. 105, 6072 (1996).

79. Jiu-Yuan Ge and John Z.H. Zhang, "Quantum mechanical tunneling through a time-dependent barrier," J. Chem. Phys. 105, 8628 (1996).

80. D.J. Kouri, D.K. Hoffman, T. Peng, and J.Z.H. Zhang, "Reactant-product decoupling for state-tostate reactive scattering: Further partitioning in the product arrangements," Chem. Phys. Lett. 262, 519 (1996).

81. Yici Zhang, Yanbing Zhang, Desheng Zhang, Qinggang Zhang, D.H. Zhang, John Z.H. Zhang, Chinese Science Bulletin, 42, 116 (1997).

82. W. Zhu, T. Peng and J.H. Z. Zhang, "Reactant-product decoupling method for state-to-state reactive scattering: A case study for 3D H + H2 exchange reaction (J= 0)," J. Chem. Phys. 106, 1742 (1997).

83. J.Z.H. Zhang, J. Dai, and W. Zhu, "Development of Accurate Quantum Dynamical Methods for Tetraatomic Reactions," (Feature article) J. Phys. Chem. 101, A, 2746 (1997).

84. J. Dai and J.H. Z. Zhang, "The application of Reactant-product Decoupling method for state-to-state calculation of D + H2 for J=0 and 1," J. Chem. Soc. Faraday Trans. 93, 699 (1997).

85. S. C. Althorpe, D. J. Kouri, D.K. Hoffman, and J.Z.H. Zhang, "Reactant-product decoupling approach to state-resolved reactive scattering: Time-independent wavepacket formulation," J.

Chem. Soc. Faraday Trans. 93, 703 (1997).

86. Q. Wu and J. Z.H. Zhang, "Perturbative approach to potential surface inversion for bound and halfscattering problems," Spectrochimica Acta Part A, 53 1189 (1997).

87. W. Zhu, D.Y.Wang, and J.Z.H. Zhang, "Quantum dynamics study of Li + HF reaction,' Theor. Chem. Acct. 96, 31 (1997).

88. D.Y. Wang, J.Z.H. Zhang, C.H. Yu, "Quantum calculation of photodetachment spectrum of OH^-(H2)," Chem. Phys. Lett. 273, 171 (1997).

89. D.Y. Wang, W. Zhu, J.Z.H. Zhang, and D.J. Kouri, "Reactant-product decoupling approach to half scattering problems: photodissociation of H2O in 3D", J. Chem. Phys. 107, 751 (1997).

90. Q. Wu, J.Z.H. Zhang, and J.M. Bowman, "Inverse perturbation via singular value decomposition: application to correction of potential surface for HCN", J. Chem. Phys. 107, 3607, (1997).

91. Da-Ren Guan, Xian Zhao, Cong-Hao Deng, and John Z.H. Zhang, "Total and partial decay width in vibrational predissociation of the HeI2 van der Waals complex for lower initial vibrational excitations," Int. J. Quant. Chem., 62, 89 (1997).

92. Da-Ren Guan, Xian Zhao, Cong-Hao Deng, and John Z.H. Zhang, "Three-dimensional quantum dynamics study of vibrational predissociation of HeI2 van der Waals molecule for low vibrational excitation using the time-dependent wave packet method," Sci. China, Ser. B: Chem. 40, 442 (1997).

93. J.Y. Ge and John Z.H. Zhang, "Use of negative complex potential as absorbing potential," J. Chem. Phys. 108, 1429 (1998).

94. W. Zhu, J.Z.H. Zhang, Y.C Zhang, Y.B. Zhang, L.X. Zhan, and S.L. Zhang, "Quantum dynamics study of H2+CN → HCN+H reaction in full dimensions," J. Chem. Phys. 108, 3509 (1998).

95. Y. Qiu, J.Z.H. Zhang, and Z. Bacic, "Six-dimensional quantum calculations of vibration-rotationtunneling levels of v1 and v2 of HCl-stretching excited (HCl)2," J. Chem. Phys. 108, 4804 (1998).

96. D.Y.Wang and J.Z.H. Zhang, "Correction of repulsive potential energy surface for photodissociation of H2O in the Ãˆ state," J. Chem. Phys. 108, 10027 (1998).

97. W. Zhu, J. Z. H. Zhang, and D. H. Zhang, "Full-dimensional Quantum Dynamics Calculation for D2 + CN Reaction, Chem. Phys. Lett. 292, 46 (1998).

98. J. Y. Ge and J. Z. H. Zhang, "Channel-dependent Complex Absorbing Potential for Multi-channel Scattering," Chem. Phys. Lett. 292, 51 (1998).

99. T. Peng, W. Zhu, D.Y. Wang, and J.Z.H. Zhang, "The Reactant-Product Decoupling Approach to State-to-State Dynamics Calculation for Bimolecular Reaction and Unimolecular Fragmentation," Faraday Discussions, No. 110, 159 (1998).

100. Y.C. Zhang, Y.B. Zhang, L.X. Zhan, S.L. Zhang, D.H. Zhang, J.Z.H. Zhang, "Time-dependent quantum dynamics study of reactive scattering of H+O2 involving long-lived resonances", Chinese Phys. Lett., 15, 16 (1998).

101. J.Z.H. Zhang, "Dissociative Chemisorption on Metal Surface," Proc. SPIE-Int. Soc. Opt. Eng. 3272, 167 (1998).

102. Y.C Zhang, L.X Zhan, Q.G Zhang,W. Zhu and J.Z.H. Zhang, "QuantumWavepacket Calculation for the Ion Molecule Reaction $N^+ + H2 \rightarrow NH^+ + H$," Chem. Phys. Lett. 300, 27 (1999).

103. D.Y. Wang, T. Peng, and J.Z.H. Zhang, W.C Chen and C.H. Yu "Quantum Dynamics from Ab Initio Points," Phys. Chem. and Chem. Phys. 1, 1067 (1999).

104. D.H. Zhang and J.Z.H. Zhang, "A uniform J-shifting approach for calculating reaction rate constant", J. Chem. Phys. 110, 7622 (1999).

105. D.H. Zhang, D.Y.Wang, T. Peng, and J.Z.H. Zhang, "Ab Initio SOFA quantum dynamics for chemical reactions", Chem. Phys. Lett. 307, 453 (1999).

106. J.Z.H. Zhang, "The semirigid vibrating rotor target model for quantum polyatomic reaction dynamics", J. Chem. Phys. 111, 3929 (1999).

107. Y.C. Zhang, L.X. Zhan, Z.M. Tan, Q.G. Zhang, and J.Z.H. Zhang "Arrangement transformation approach to state-to-state quantum reactive scattering of H+DH → DH+H, HH+D", SCIENCE IN CHINA SERIES, 42, 973-979 (1999).

108. D.H. Zhang and J.Z.H. Zhang, "Quantum Wavepacket Approach to Chemical Reaction Dynamics: perspective on Dynamics of the Collinear H + H2 Reaction. I. Probability Density and Flux by E.A. McCullough, Jr. and R.E. Wyatt [J. Chem. Phys. vol. 54, 3578 (1971)]", Theor. Chem. Acct. 103, 300 (2000).

109. D.H. Zhang and J.Z.H. Zhang, "The semirigid vibrating rotor target model for atom-polyatom reaction: Application to H + H2O reaction", J. Chem. Phys. 112, 585 (2000).

110. S.Y. Lin, K.L. Han, J.Z.H. Zhang, "Accurate quantum-mechanical calculation for O(1D)+DCl reaction", Chem. Phys. Lett. 324, 122-126 (2000).

111. S.Y. Lin, K.L. Han, and John Z. H. Zhang "Time-dependent wavepacket study for O(1D)+HCl (v0=0, j0=0) reaction" Phys. Chem. and Chem. Phys. 2, 2529-2534 (2000).

112. T. Peng, D.H. Zhang, D.Y. Wang, Y.M. Li, and J.Z.H. Zhang, "Dynasol: A visual quantum dynamics package", Comput. Phys. Commun. 128, 492 (2000).

113. S. Zhang, Z. Tan, H. Zhang, Y. Zhang, and J.Z.H. Zhang, "Reactant-product decoupling approach to state-to-state reactive scattering H + DH", Chem. Phys. 255, 397 (2000).

114. M.L. Wang, Y. Li, J.Z.H. Zhang, and D.H. Zhang, "Application of semirigid vibrating rotor target model to reaction of H + CH4 -> CH3 + H2", J. Chem. Phys. 113, 1802 (2000).

115. B.Y. Tang, B.H. Yang, L. Zhang, K.L. Han, J.Z.H. Zhang, "Stereodynamics studies of the Sr

plus HF reaction using time-dependent quantum wave packet method", Chem. Phys. Lett. 327, 381-388 (2000).

116. B.H. Yang H.T. Gao, K.L. Han, J.Z.H. Zhang "Time-dependent quantum dynamics study of the Cl + H2 reaction", J. Chem. Phys. 113, 1434-1440 (2000).

117. S.Y. Lin, K.L. Han, J.Z.H. Zhang "Accurate quantum-mechanical calculation for O(D-1)+DCl reaction", Chem. Phys. Lett. 324, 122-126 (2000).

118. Y.C. Zhang, Z.M. Tan, H.Y. Zhang, Q.G. Zhang, J.Z.H. Zhang, "Time-dependent quantum dynamics study of reactive scattering of the HD plus CN system in the potential averaged 5D model", Chem. Phys. 252, 191-197 (2000).

119. B.H. Yang, B.Y. Tang, H.M. Yin, K.L. Han, and J.Z.H. Zhang, "Quantum dynamics study of the Cl + D2 reaction: Time-dependent wave packet calculations" J. Chem. Phys. 113, 7182, (2000).

120. B.Y. Tang, B.H. Yang, K.L. Han, R.Q. Zhang, and J.Z.H. Zhang, "Time-dependent quantum wave packet studies of the F+HCl and F+DCl reactions" J. Chem. Phys. 113, 10105, (2000).

121. B.H Yang, H.M. Yin, K.L. Han, and J.Z.H. Zhang, "Time-Dependent Quantum Dynamics Study of the Cl + HD Reaction", J. Phys. Chem. A 104, 10517 (2000).

122. M.L. Wang, Y.M. Li, and J.Z.H. Zhang, "Application of semirigid vibrating rotor target model to the reaction of O(3P) + CH4 → CH3 + OH reaction", J. Phys. Chem. A 105, 2530 (2001).

123. Y.M. Li, M.L. Wang, J.Z.H. Zhang, and D.H. Zhang, "SVRT calculation for reaction H + HOD →H2+OD, HD + OH", J. Chem. Phys. 114, 7013 (2001)

124. B.Y. Tang, M.D. Chen, K.L. Han, and J.Z.H. Zhang, "Time-dependent quantum wavepacket study of the C + CH reactant", J. Chem. Phys. 115, 731 (2001).

125. Yici Zhang, Jingfeng Zhang, Haiyan Zhang, Qinggang Zhang, John Z.H. Zhang, "Time-dependent wavepacket calculation for state-to-state reaction of Cl + H2 using the reactant-product decoupling (RPD) approach", J. Chem. Phys. 115, 8455 (2001).

126. B.Y. Tang, M.D. Chen, K.L. Han, and J.Z.H. Zhang, "Time-dependent quantum dynamics study of the C plus CH reaction on the 2A ' surface", J. Phys. Chem. A 105, 8629 (2001).

127. M.L. Wang and J. Z. H. Zhang, "Stereodynamics and rovibrational effect for H + CH4(v,j,K,n) → H2 + CH3 reaction", J. Chem. Phys. 116, 6497; 117 10425 (erratum) (2002).

128. X. Zhang, K.L. Han and J.Z.H. Zhang, "SVRT calculation for bond-selective reaction H+HOD > H-2+OD, HD+OH", J. Chem. Phys. 116, 10197 (2002).

129. W.Y. Ma, K.L. Han KL, M.L.Wang and J.Z.H. Zhang, "Time-dependent quantum wave packet study of H+HCN→H-2+CN reaction", J. Chem. Phys. 117, 172 (2002).

130. M.L. Wang and J. Z. H. Zhang, "Generalized semirigid vibrating rotor target model for atom-poly reaction: Inclusion of umbrella mode for H+CH4 reaction", J. Chem. Phys. 117,

3081, 10426 (erratum) (2002).

131. Yi M. Li and J. Z. H. Zhang, "Quantitative Quantum Dynamics Calculation of H2 + CH3 -> H + CH4 Reaction", J. Theo. and Comput. Chem. 1, 25 (2002).

132. Y. Xiang, J.Z.H. Zhang and D.Y. Wang, "Semirigid vibrating rotor target model for CH4 dissociation on a Ni(111) surface", J. Chem. Phys. 117, 7698 (2002).

133. W.Y. Ma, K.L. Han and J.Z.H. Zhang, "Time-dependent quantum wave packet study of the H+DCN → HD+CN reaction", J. Chem. Phys. 117, 5642-5646 (2002).

134. M.D Chen, B.Y. Tang, K.L. Han, N.Q. Lou and J.Z.H. Zhang, "Accurate quantum mechanical calculation for the N+OH reaction," J. Chem. Phys. 118, 6852-6857 (2003).

135. D.W. Zhang, M.L. Wang and J.Z.H. Zhang, "Ab initio quantum dynamics study of rotationally inelastic scattering of glycine by hydrogen atom," J. Chem. Phys. 118, 2716-2722 (2003).

136. M.L. Wang and J.Z.H. Zhang, "Mixed quantum-classical study of energy transfer in a Na+ collision with a peptide," J. Chem. Phys. 118, 7846 (2003).

137. D.W. Zhang, M.L. Wang and J.Z.H. Zhang, "Quantum dynamics study of torsional excitation of glycine in collision with hydrogen atom on ab initio potential energy surface," J. Phys. Chem. A 107, 7106-7111(2003).

138. Y. Xiang and J.Z.H. Zhang, "A mixed quantum-classical semirigid vibrating rotor target approach to methane dissociation on Ni surface," J. Chem. Phys. 118, 8954 (2003).

139. Xin Zhang, Guang-Hui Yang, and Ke-Li Han, M.L. Wang, and J.Z.H. Zhang, "Quantum dynamics study of isotope effect for H + CH4 eaction using the SVRT model," J. Chem. Phys. 118, 9266 (2003).

140. D.W. Zhang, Yi M. Li and J.Z.H. Zhang, "Local linear least square fitting of potential energy surface", J. Theo. and Comput. Chem. 2, 119 (2003).

141. D.W. Zhang and J.Z.H. Zhang, "Molecular fractionation with conjugate caps for full quantum mechanical calculation of protein-molecule interaction energy", J. Chem. Phys. 119, 3599 (2003).

142. D.W. Zhang, X.H. Chen, and J.Z.H. Zhang, "Molecular caps for full quantum mechanical computation of peptide-water interaction energy", J. Comput. Chem. 24, 1846 (2003).

143. Qian Cui, Xiao He, Ming-Liang Wang, and J.Z.H. Zhang, "Comparison of quantum and mixed quantum-classical SVRT studies for isotopic reactions H(D,T) + CH4 → HH(D,T) + CH3", J. Chem. Phys. 119, 9455 (2003).

144. Ming-liang Wang and John Z.H. Zhang, "Mixed Quantum-classical Semi-rigid Vibrating Rotor Target Model for Atom-Polyatom Reaction: O(3P) + CH4 → CH3 + OJ", J. Theo. and Comput. Chem. 2, 351 (2003).

145. D.W. Zhang, Yun Xiang, and John Z.H. Zhang, "New advance in computational chemistry:

full quantum mechanical ab initio computation of streptavidin-biotin interaction energy", J. Phys. Chem. B 107, 12039 (2003).

146. MingliangWang and J.Z.H. Zhang, "Mixed quantum-classical study of energy transfer between H2O and dipeptide", J. Chem. Phys. 119, 11152 (2003).

147. Yan Zhang, Ting-Xian Xie, K.L. Han, and J.Z.H. Zhang, "Time-dependent quantum wavepacket calculation for nonadiabatic F(2P3/2,2P1/2) + H2 reaction", J. Chem. Phys. 119, 12921 (2003).

148. D.W. Zhang and J.Z.H. Zhang, "Full quantum mechanical ab initio computation of protein-molecule interaction energies", J. Theo. and Comput. Chem. 3, 43-49 (2004).

149. X.H. Chen, D.W. Zhang, and J.Z.H. Zhang, "Fractionation of peptide with disulfide bond for quantum mechanical calculation of interaction energy with molecules", J. Chem. Phys. 120, 839-844 (2004).

150. D.W. Zhang, Y. Xiang, A.M. Gao and J.Z.H. Zhang, "Quantum mechanical map for protein-ligand binding with application to beta-trypsin/benzamidine complex", J. Chem. Phys. 120, 1145 (communication) (2004).

151. Yan Zhang, Ting-Xian Xie, Ke-Li Han, and J.Z.H. Zhang, "The investigation of spin orbit effect for the F(2P)+HD reaction", J. Chem. Phys. 120, 6000 (2004)

152. J. Z. H. Zhang, Yi M. Li, Ming L.Wang and Yun Xiang, "Theoretical Dynamics Treatment of Chemical Reactions", in Modern Trends in Chemical Reaction Dynamics, Part I: Experiment and Theory, ed., Xueming Yang and Kopin Liu, (World Scientific Publishing, Singapore, 2004), p. 209.

153. X.H. Chen and J.Z.H. Zhang, "Theoretical method for full ab initio calculation of DNA/RNA-ligand interaction energy", J. Chem. Phys. 120, 11386-11391 (2004).

154. Y. Xiang, D.W. Zhang, John Z.H. Zhang, "Fully Quantum Mechanical Energy Optimization for Protein-Ligand Structue", J. Comput. Chem. 25, 1431-1437(2004).

155. B.Y. Tang, Q.K. Tang, M.D. Chen, K.L. Han, J.Z.H. Zhang, "Quantum scattering calculation of the O(D-1) plus HBr reaction", J. Chem. Phys. 120, 8537-8543 (20 04).

156. L. Yao, K.L. Han, H.S. Song, J.Z.H. Zhang, "The semirigid vibrating rotor target model for atom-polyatom reaction: Application to F+CH2D2→CH2D/CHD2+DF/HF", Chin. J. Chem. Phys. 17, 339-345 (2004).

157. Ai M. Gao, D.W. Zhang, John Z.H. Zhang and Yingkai Zhang, "An efficient linear scaling method for ab initio calculation of electron density of proteins" Chem. Phys. Lett. 394, 293-297 (2004).

158. Liu XG, Zhang QG, Zhang YC, et al. "Time-dependent quantum dynamics study for reaction of D+CH4→ CH3+HD", Chin. Phys. 13, 1013-1017 (2004).

159. X. H. Chen and J. Z. H. Zhang, "MFCC-Downhill simplex method for molecular structure optimization", J. Theo. and Comput. Chem. 3, 277 (2004).

160. Mei-Yu Zhao, Ke-Li Han, Guo-Zhong He and John Z. H. Zhang, "Photodissociation of ozone in the Hartley band: fragment rotational quantum state distributions", J. Theo. and Comput. Chem. 3, 443 (2004).

161. D.W. Zhang and J.Z.H. Zhang, "Full quantum mechanical study of binding of HIV-1 protease drugs", Int. J. Quant. Chem. 103, 246-257 (2005).

162. Y. Mei, D.W. Zhang, and J.Z.H. Zhang, "A new method for direct linear scaling calculation of electron density of protein", J. Phys. Chem. A 109, 2 (2005) (Letter)

163. Xiao He and John Z.H. Zhang, "A new method for direct calculation of total energy of protein", J. Chem. Phys. 122, 031103 (2005) (communication).

164. Y. Mei, X. He, Y. Xiang, D.W. Zhang, and J.Z.H. Zhang, "Quantum study of mutational effect in binding of Efavirenz to HIV-1 RT", Proteins: Structure, Function and Bioinformatics 59, 489-495 (2005).

165. X. He, Y. Mei, Y. Xiang, D.W. Zhang, and J.Z.H. Zhang, "Quantum computational analysis for drug resistance of HIV-1 reverse transcriptase to nevirapine through point mutations", Proteins: Structure, Function and Bioinformatics 61, 423-432 (2005).

166. Xi Hua Chen, Yingkai Zhang, and John Z.H. Zhang, "An efficient approach for energy calculation of biopolymers", J. Chem. Phys. 122, 184105 (2005).

167. Q. Cui, M.L. Wang, J.Z.H. Zhang, "Effect of entrance channel topology on reaction dynamics: O+CH4 -> CH3O + H4", Chem. Phys. Lett. 410,115-119 (2005).

168. L.P. Ju, K.L. Han, and J.Z.H. Zhang, "A theoretical study for H-2+CN ←→ HCN+H reaction and its kinetic isotope effects with variational transition state theory", J. Theo. & Comput. Chem.: 5, 769-777 (2006).

169. Ye Mei, Emilia L. Wu, K.L. Han, and J.Z.H. Zhang, "Treating hydrogen bonding in ab initio calculation of biopolymers," *Int. J. Quant. Chem.* 106, 1267-1276 (2006).

170. Y. Zhang, T.X. Xie, K.L. Han, J.Z.H. Zhang, "Nonadiabatic reactant-product decoupling calculation for the F(2P1/2)+H2 reaction", *J. Chem. Phys.* 124, 134301 (2006).

171. X. He and J.Z.H. Zhang, "The generalized molecular fractionation with conjugate caps/molecular mechanics method for direct calculation of protein energy", *J. Chem. Phys.* 124, 184703 (2006).

172. T.S. Chu, X. Zhang, L.P. Ju, L. Yao, K.L. Han, M.L. Wang, J.Z.H. Zhang, "First principles quantum dynamics study reveals subtle resonance in polyatomic reaction: The case of F+CH4→HF+CH3", *Chem. Phys. Lett.* 424, 243-246 (2006).

173. S.A. Vail, D.I. Schuster, D.M. Guldi, M. Isosomppi, N. Tkachenko, H. Lemmetyinen, A. Palkar, L. Echegoyen, X.H. Chen, J.Z.H. Zhang, "Energy and electron transfer in beta-alkynyl-linked porphyrin-[60]fullerene dyads", *J. Phys. Chem. B* 110, 14155-14166 (2006).

174. X.H. Chen and J.Z.H. Zhang, "Molecular fractionation with conjugated caps density matrix with pairwise interaction correction for protein energy calculation", *J. Chem. Phys.* 125,

044903 (2006).

175. J. C. Varandas, P. J. S. B. Caridade, J. Z. H. Zhang, Q. Cui, and K. L. Han, "Dynamics of X+CH4 (X=H, O, Cl) reactions: How reliable is transition state theory for fine-tuning potential energy surfaces?", *J. Chem. Phys.* 125, 064312 (2006).

176. Y. Mei, C.G. Ji, and J.Z.H. Zhang, "A new quantum method for electrostatic solvation energy of protein," *J. Chem. Phys.* 125, 094906 (2006),

177. R.F. Lu, T.S. Chu, Y. Zhang, and K.L. Han, A.J.C. Varandas, and J.Z.H. Zhang, "Nonadiabatic effects in the H+D2 reaction," *J. Chem. Phys.* 125, 133108 (2006).

178. Y.S. Wang, S. Sabu, S.C. Wei, C.M.J. Kao, X.L. Kong, S.C. Liau, C.C. Han, H.C. Chang, S.Y. Tu, A.H. Kung, J.Z.H. Zhang, "Dissociation of heme from gaseous myoglobin ions studied by infrared multiphoton dissociation spectroscopy and Fourier-transform ion cyclotron resonance mass spectrometry", *J. Chem. Phys.* 125, 133310 (2006).

179. S. Lee-Huang, P.L. Huang, D. Zhang, J.W. Lee, J. Bao, Y. Sun, Y-Tae Chang, J. Zhang and P. L. Huang, "Discovery of small-molecule HIV-1 fusion and integrase inhibitors oleuropein and hydroxytyrosol: Part I. Fusion inhibition", *Biochem. Biophys. Res. Commun.* 354, 872-878 (2007).

180. S. Lee-Huang, P.L. Huang, D. Zhang, J.W. Lee, J. Bao, Y. Sun, Y-Tae Chang, J.Z.H. Zhang and P. L. Huang, "Discovery of small-molecule HIV-1 fusion and integrase inhibitors oleuropein and hydroxytyrosol: Part II. Integrase inhibition", *Biochem. Biophys. Res. Commun*. 354, 879-884 (2007).

181. Emilia L. Wu, Ye Mei, Ke L. Han, and John Z.H. Zhang, "Quantum computational study for binding of Oscillarin and two Macrocyclic inhibitors to human alpha thrombin using the MFCC method", *Biophys. J.* 92, 4244 (2007).

182. Xu Q. Zhang, Q. Cui, Ke L. Han, J.Z.H. Zhang, "Quantum dynamics study of H + NH3 → H2 + NH2 reaction", *J. Chem. Phys.* 126, 234304 (2007).

183. L.L. Duan, Y. Tong, Y. Mei, Q.G. Zhang, J. Z.H. Zhang, "Quantum study of HIV-1 protease-bridge water interaction", *J. Chem. Phys.* 127, 145101 (2007).

184. J. Bao, D. W. Zhang, J. Z.H. Zhang, P. L. Huang, P.L. Huang, S. Lee-Huang, "Computational study of bindings of olive leaf extract (OLE) to HIV-1 fusion protein gp41", *FEBS Letters* 581, 2737-2742 (2007).

185. Xi-Hua Chen and John Z. Zhang, "A non-derivative MFCC optimization study of cyclohexapeptide monohydrate", *Chinese J. Chem. Phys*. 20, 431 (2007).

186. Yun Ding, Ye Mei, John Z.H.Zhang, and Fu-ming Tao, "Efficient bond function basis set for pi-pi interaction energies", *J. Comput. Chem.* 29, 275 (2008).

187. C.G. Ji, Y. Mei and J.Z.H. Zhang, "Developing polarized protein-specific charges for protein dynamics: MD free energy calculation of pKa shifts for Asp26/Asp20 in thioredoxin", *Biophysical Journal* **95**, 1080 (2008).

188. E.L. Wu, K.L. Han and J.Z.H. Zhang, "Molecular Dynamics Study for the selectivity of Neutral/ Weakly Basic P1 groups inhibitors with Thrombin and Trypsin", *Chemistry-A European Journal* **14**, 8704-8714 (2008)..

189. Y. Ding, Y. Mei, J.Z.H. Zhang, "Quantum mechanical studies of residue-specific hydrophobic interactions in p53-MDM2 binding", *J. Phys. Chem. B* **112**, 11396-401 (2008).

190. D.W. Zhang, P.L. Huang, S. Lee-Huang, "Design of hybrid inhibitors to HIV-1 protease", *J. Theo. & Comput. Chem.* **7**, 485 (2008).

191. C.G. Ji and J.Z.H. Zhang, "Protein Polarization Is Critical to Stabilizing AF-2 and Helix-2' Domains in Ligand Binding to PPAR gamma", *J. Am. Chem. Soc. 1*30, 17129–17133 (2008).

192. M. Han and J.Z.H. Zhang, "Molecular Dynamic Simulation of Kv1.2 Voltage-gated Potassium Channel in Open and Closed State Conformations", *J. Phys. Chem. B 112*, 16966–16974 (2008).

193. L.L. Duan, Y. Mei, Q.G. Zhang, and J.Z.H. Zhang, "Intra-protein hydrogen bonding is dynamically stabilized by electronic polarization", *J. Chem. Phys. 130*, 115102 (2009).

194. Li-Ping Ju, K.L. Han, J. Z.H. Zhang, "Global Dynamics and Transition State Theories: Comparative Study of Reaction Rate Constants for Gas-Phase Chemical Reactions", *J. Comput. Chem. 30*, 305-316 (2009).

195. Y. Tong, C.G. Ji, Y. Mei, J.Z.H. Zhang, "Simulation of NMR Data Reveals that Protein's local structures Are Stabilized by Electronic Polarization", *J. Am. Chem. Soc.* 131, 8636–8641 (2009).

196. J. Bao, X.Y. Dong, J.Z.H. Zhang, P.S. Arora, "Dynamical Binding of Hydrogen-Bond Surrogate Derived Bak Helices to Antiapoptotic Protein Bcl-x(L)", *J. Phys. Chem. B* 113, 3565-3571 (2009).

197. E.L. Wu, K.L. Han, J.Z.H. Zhang, "Computational Study for Binding of Oscillarin To Human Alpha-Thrombin", *J. Theo. & Comput. Chem.* 8, 551-560 (2009).

198. C.G. Ji and J.Z.H. Zhang, "NMR Scalar Coupling Constant Reveals That Intraprotein Hydrogen Bonds Are Dynamically Stabilized by Electronic Polarization", J. *Phys. Chem. B*, 113, 13898-13900 (2009).

199. C.G. Ji and J.Z.H. Zhang, "Electronic Polarization Is Important in Stabilizing the Native Structures of Proteins," J. *Phys. Chem. B*, 113, 16059–16064 (2009).

200. Y. Mei and J.Z.H. Zhang, "Numerical Stabilities in Fitting Atomic Charges to Electric Field and Electrostatic Potential", *J. Theo. Comput. Chem.* 8, 925-942 (2009).

201. Y.L. Li, L. Han, Y. Mei, and J.Z.J. Zhang, "Time-dependent density functional theory study of absorption spectra of metallocenes", *Chem. Phys. Letts.* 482, 217-222 (2009).

202. Y. Tong, Y. Mei, J.Z.H. Zhang, L.L. Duan, Q.G. Zhang, "Quantum calculation of protein solvation and protein–ligand binding free energy for hiv-1 protease/water complex", *J. Theo. Comput. Chem.* 8, 1265-1279 (2009).

203. H.G. Li, P.L. Huang, D.W. Zhang, Y.T. Sun, H.C. Chen, J. Zhang, P.L. Huang, X.P. Kong, S. Lee-Huang, "A new activity of anti-HIV and anti-tumor protein GAP31: DNA adenosine glycosidase - Structural and modeling insight into its functions", *Biochem. Biophys. Res. Commun.*, 391, 340-345 (2010).

204. M. Han and J.Z.H. Zhang, "Class I Phospho-inositide-3-kinases (PI3Ks) Isoform-Specific Inhibition Study by the Combination of Docking and Molecular Dynamics Simulation", *J. Chem. Info. Mod.* 50, 136-145 (2010).

205. Y. Tong, Y. Mei, Y.L. Li, C.G. Ji, J.Z.H. Zhang, "Electrostatic polarization makes substantial contribution to free energy of avidin-biotin binding", *J. Am. Chem. Soc.* 132, 5137-5142 (2010).

206. Yunpeng Lu, Y. Mei, J.Z.H. Zhang, Dawei Zhang, "Electron polarization critically stabilizes the Mg^{2+} complex in the catalytic core domain of HIV-1 integrase", *J. Chem. Phys.* (Communications), 132, 131101 (2010).

207. L.L. Duan, Y. Mei, Y.L. Li, Q.G. Zhang, D.W. Zhang, J.Z.H. Zhang, "Simulation of the thermodynamics of folding and unfolding of the Trp-cage mini-protein TC5b using different combinations of force fields and solvation models", *Science China-Chemistry* **53**, 196-201 (2010).

208. Li L. Duan,Ye Mei,Dawei Zhang, Qing G. Zhang, and John Z. H. Zhang, "Folding of a Helix at Room Temperature Is Critically Aided by Electrostatic Polarization of Intraprotein Hydrogen Bonds", *J. Am. Chem. Soc*. 132, 11159–11164 (2010).

209. P. Wang and J.Z.H. Zhang, "Selective Binding of Anti-influenza Drugs and Their Analogues to 'Open' and 'Closed' Conformations of H5N1 Neuraminidase", *J. Phys. Chem. B* 114, 12958-12964 (2010).

210. D.W. Zhang, L.Z. Yu, P.L. Huang, P.L. Huang, S. Lee-Huang, J.Z.H. Zhang, "COMPUTATIONAL DESIGN OF NORBORNANE-BASED HIV-1 PROTEASE INHIBITORS", *J. Theo. Comput. Chem.* 9, 471-485 (2010).

211. Y. Xiang, L.L. Duan, J.Z.H. Zhang, "Folding dynamics of a small protein at room temperature via simulated coherent two-dimensional infrared spectroscopy", *Phys. Chem. Chem. Phys.* 12, 15681-15688 (2010).

212. X. Y. Wang and J.Z.H. Zhang, "Effect of polarization on the stability of a helix dimer", *Chem. Phys. Lett.* 501, 508-512 (2011).

213. Y. Xiang, L.L. Duan, J.Z.H. Zhang, "Protein's electronic polarization contributes significantly to its catalytic function", *J. Chem. Phys.* **134**, 205101 (2011).

214. Y. L. Li, Yong, Y. Mei, D.W. Zhang, D.Q. J.Z.H. Zhang, "Structure and Dynamics of a Dizinc Metalloprotein: Effect of Charge Transfer and Polarization", *J. Phys. Chem. B* 115, 10154-10162 (2011).

215. K.Z. Song, J. Bao, Y.M. Sun, J.Z.H. Zhang, "Computational Characterization of Binding of Small Molecule Inhibitors to HIV-1 gp41", *Chin. J. Chem*. 29, 1307-1311 (2011).

216. C.G. Ji and J.Z.H. Zhang, “Quantifying the Stabilizing Energy of the Intra-protein Hydrogen Bond Due to Local Mutation”, *J. Phys. Chem. B* **115**, 12230–12233 (2011).

217. C.G. Ji and J.Z.H. Zhang, “Understanding the Molecular Mechanism of Enzyme Dynamics of Ribonuclease A through Protonation/Deprotonation of HIS48”, *J. Am. Chem. Soc*. **133**, 17727-17737 (2011).

218. Y. Mei, D.W. Zhang, L.L. Duan, etc., “Folding of EK peptide and its dependence on salt concentration and pH: A computational study”, *Science China-Chemistry*, 54, 1974-1981 (2011).

219. Y. Gao, Lu, X. L., Duan, L. L., Zhang, J. Z. H, Mei, Y., “Polarization of Intraprotein Hydrogen Bond Is Critical to Thermal Stability of Short Helix”, *J. Phys. Chem. B*, 2011, 116, 1 549-554 (2012).

220. Tong Zhu, Xiao He and John Z.H. Zhang, “Fragment density functional theory calculation of NMR chemical shift for proteins with implicit salvation”, *Phys. Chem. Chem. Phys.* 14, 7837 (2012).

221. L.L. Duan, Y. Gao, Y. Mei, Q.G. Zhang, B. Tang, J.Z.H. Zhang, “Folding of a Helix is Critically Stabilized by Polarization of Backbone Hydrogen Bonds: Study in Explicit Water”, *Journal of Physical Chemistry B*, 116, 3430 (2012).

222. Ya Gao, Guo, M.， Ye Mei, and John Z.H. Zhang, “Protein-Water Hydrogen Bonds are Stabilized by Electrostatic Polarization”, *Molecular Physics*, 110, 595 (2012).

223. C.G. Ji and J.Z.H. Zhang, “Effect of inter-protein polarization on protein-protein binding energy”, *J. Comput. Chem.*, 33, 16, 1416–1420（2012）.

224. Ye Mei, Yong L. Li, Juan Zeng, and John Z.H. Zhang, “Electrostatic polarization is critical for the strong binding in streptavidin-biotin system”, *J. Comput. Chem.*, 33, 1374 (2012).

225. Ye Mei, Xiao He, Chang G. Ji, and John Z.H. Zhang, “A Fragmentation Approach to Quantum Calculation of Large Molecular Systems”, *Progress in Chemistry*, 24, 1058 (2012).

226. Weixin Xu, Li Yang; Zhang, John Z. H.，"Calculation of Collective Variable-based PMF by Combining WHAM with Umbrella Sampling"，*Chinese Physics Letters*, Vol. 29, 068702, (2012) .

227. Weixin Xu, Haibin Su, John Z. H. Zhang, Yuguang Mu, Molecular Dynamics Simulation Study on the Molecular Structures of the Amylin Fibril Models, *J. Phys. Chem. B*, 116，13991-13999, 2012

228. Chang G. Ji, Xudong Xiao, and John Z. H. Zhang, "Studying the Effect of Site-Specific Hydrophobicity and Polarization on Hydrogen Bond Energy of Protein Using a Polarizable Method",*J. Chem. Theory Comput.*, *8* (6), pp 2157–2164(2012).

229. Mei, Y.,Wei, C. Y.,Yip, Y. M.,Ho, C. Y., Zhang, J. Z. H., Zhang, D. W., “Folding and thermodynamic studies of Trp-cage based on polarized force field”, *Theoretical Chemistry Accounts*, 131, 1168 (2012).

230. Jiang, Biao,Han, Lei, Li, Yong-Le, Xiao-Long Zhao, Yang Lei, Dai-Qian Xie,and John Z. H. Zhang, "Combined Theoretical and Experimental Study on High Diastereoselective Chirality Transfer Based on [2.2]Paracyclophane Derivative Chiral Reagent", *Journal of Organic Chemistry* ,77 , 4 , 1701-1709 (2012).

231. Jun Xu, John Z. H. Zhang, and Yun Xiang, "Ab Initio QM/MM Free Energy Simulations of Peptide Bond Formation in the Ribosome Support an Eight-Membered Ring Reaction Mechanism"， *J. Am. Chem. Soc.*, 134, 16424−16429 (2012)

232. Xing Y. Wang, Chang G. Ji, and John Z. H. Zhang， "Exploring the Molecular Mechanism of Stabilization of the Adhesion Domains of Human CD2 by N-Glycosylation"， *J. Phys. Chem. B, 116* (38), pp 11570–11577（2012).

233. Yang Li , Changge Ji , Weixin Xu , and John Z.H. Zhang ,"Dynamical Stability and Assembly Cooperativity of β-Sheet Amyloid Oligomers – Effect of Polarization", *J. Phys. Chem. B*, 116, 13368–13373（2012).

234. X. Xiao, T. Zhu, C.G Ji, J.Z.H. Zhang, "Development of an Effective Polarizable Bond Method for Biomolecular Simulation", J. Phys. Chem. B 117 (48), 14885-14893 (2013).

235. J.N. Song, C.G. Ji, and J.Z.H. Zhang, "Unveiling the gating mechanism of ECF Transporter RibU", Scientific Reports, 3, 3566 (2013).

236. Ren, S., Zeng, J., Mei, Y., Zhang, J. Z. H., Yan, S. F., Fei, J.,Chen, L., "Discovery and characterization of novel, potent, and selective cytochrome P450 2J2 inhibitors", Drug Metabolism and Disposition, 41, 60-71 (2013)

237. S.Y. Lin, P.Y. Zhang, J.Z.H. Zhang, "Hybrid many-body-expansion/Shepard-interpolation method for constructing ab initio potential energy surfaces for quantum dynamics calculations", Chem. Phys. Letts., 556, 393-397 (2013).

238. Jianing Song, C.G. Ji, J.Z.H. Zhang, "The critical effect of polarization on the dynamical structure of guanine quadruplex DNA", Phys. Chem. Chem. Phys., 15, 3846-3854 (2013).

239. Z. Juan; Duan, Li Li; Zhang, John Z. H., Y. Mei, "A numerically stable restrained electrostatic potential charge fitting method", J. Comput. Chem. 34(10), 847-853 (2013). .

240. Zhang, SQ , Mu, YG ,Zhang, JZH ; ,Xu, WX , "Effect of Self-Assembly of Fullerene Nano-Particles on Lipid Membrane, PLOS ONE , 8,10 (2013).

241. Lu, XL ; Zeng, J ; Gao, Y ; Zhang, JZH; Zhang, DW ; Mei, Y , "The intrinsic helical propensities of the helical fragments in prion protein under neutral and low pH conditions: a replica exchange molecular dynamics study", J. Mol. Model., 19 ,4897-4908 (2013).

242. Zeng, J ;Jia, XY ;Zhang, JZH; Mei, Y, "The F130L Mutation in Streptavidin Reduces Its Binding Affinity to Biotin through Electronic Polarization Effect", J. Comput. Chem., 34, 2677-2686 (2013).

243. Yang Li; Weixin Xu; Yuguang Mu; John Z. H. Zhang, "Acidic pH retards the fibrillization of human islet amyloid polypeptide due to electrostatic repulsion of histidines". J. Chem. Phys. 139, 5 (2013).

244. Xu, Weixin; Zhang, Ce; Morozova-Roche, Ludmilla; Mu, Yuguang; Zhang, John Z. H., "pH-Dependent Conformational Ensemble and Polymorphism of Amyloid-beta Core Fragment", J. Phys. Chem. B. 117, 8392-8399 (2013).

245. Li, Y. X.; Gao, Y.; Zhang, X. Q.; Wang, X. Y.; Mou, L. R.; Duan, L. L.; He, X.; Mei, Y.; Zhang, J.Z.H., "A coupled two-dimensional main chain torsional potential for protein dynamics: generation and implementation", J. Mol. Model., 29, 3647-3657 (2013).

246. J. Bao, J.F. Liu, X.He; J.Z.H. Zhang," Computational Study of HIV-1 gp41 NHR trimer: Inhibition Mechanisms of N-Substituted Pyrrole Derivatives and Fragment-Based Virtual Screening", J. Theor. Comput. Chem., 12(6), 13411 (2013).

247. Ya Gao; Xiaoliang Lu; Lili Duan; Dawei, Zhang; Ye, Mei; John, Z. H. Zhang, "Direct folding simulation of a long helix in explicit water". Appl. Phys. Lett. 102,193706 (2013).

248. Liu, Jinfeng; He, Xiao; Zhang, John Z. H., "Improving the Scoring of Protein-Ligand Binding Affinity by Including the Effects of Structural Water and Electronic Polarization". J. Chem. Inf. Model. 53(6), 1306-1314 (2013).

249. Xu, J, Zhang, J.Z.H., Xiang, Y, "Molecular Dynamics Simulation and Computational Two-Dimensional Infrared Spectroscopic Study of Model Amyloid beta-Peptide Oligomers", J. Phys. Chem. A, 117, 6373-6379 (2013).

250. Yao Xue Xia; Ji Chang Ge; Xie Dai Qian; Zhang, John Z. H. , "Interaction specific binding hotspots in endonuclease colicin-immunity protein complex from MD simulations". Sci. China. Chem. 56, 1143-1151 (2013).

251. Wang, XW ; He, X ; Zhang, J.Z.H.," Predicting Mutation-Induced Stark Shifts in the Active Site of a Protein with a Polarized Force Field", J. Phys. Chem. A, 117, 6015-6023 (2013)

252. Duan, L. L.; Zhu, T.; Mei, Y.; Zhang, Q. G.; Tang, B.; Zhang, J. Z. H., "An implementation of hydrophobic force in implicit solvent molecular dynamics simulation for packed proteins". J. Mol. Model., 19, 2605-2612 (2013).

253. Wang, XW ; Liu, JF ;Zhang, JZH; He, X," Electrostatically Embedded Generalized Molecular Fractionation with Conjugate Caps Method for Full Quantum Mechanical Calculation of Protein Energy", J. Phys. Chem. A, 32, 7149-7161 (2013).

254. T. Zhu, J.Z.H. Zhang and X. Xiao," Automated Fragmentation QM/MM Calculation of Amide Proton Chemical Shifts in Proteins with Explicit Solvent Model". J. Chem. Theory Comput. 9, 2104 (2013),

255. Zhu, T ; Xiao, XD ; Ji, CG ; Zhang, J.Z.H., "A New Quantum Calibrated Force Field for Zinc-Protein Complex", J. Chem. Theory Comput.,9, 1788-1798 (2013).

256. Jia, Xiangyu; Zhang, John Z. H.; Mei, Ye, "Assessing the accuracy of the general AMBER force field for 2,2,2-trifluoroethanol as solvent", J. Mol. Model., 19, 2355-2361 (2013).

257. Yao, Xue X.; Ji, Chang G.; Xie, Dai Q.; Zhang, John Z. H.,"Molecular dynamics study of DNA binding by INT-DBD under a polarized force field", J. Comput. Chem., 34, 1136-1142 (2013).

258. Xiangyu Jia, Xianwei Wang, Jinfeng Liu, John Z. H. Zhang, Ye Mei，and Xiao He, “An improved fragment-based quantum mechanical method for calculation of electrostatic solvation energy of proteins”, J. Chem. Phys., 139, 214104 (2013).

259. Li Yongxiu; Zhang J.Z.H; Mei Ye, "Molecular Dynamics Simulation of Protein Crystal with Polarized Protein-Specific Force Field". J. Phys. Chem. B. 118, 12326(2014).

260. Duan LL; Gao Y; Ji CG; Mei Y; Zhang QG; Tang B; Zhang John Z.H., "Energetics of protein backbone hydrogen bonds and their local electrostatic environment". Sci. China-Chemistry. 57, 1708-1715 (2014).

261. Min Li; Weixin Xu; John Z.H. Zhang; Fei Xia, "Combined effect of confinement and affinity of crowded environment on conformation switching of adenylate kinase". J. Mol. Model. 20, 2530 (2014).

262. Wang Xianwei; Li Yongxiu; He Xiao; Chen SD; Zhang, John, JZH, "Effect of strong electric field on the conformational integrity on insulin", J. Phys. Chem. A. 118(39). 8942-8952 (2014).

263. Liu,Jinfeng; He Xiao; Zhang, John Z. H., "Novel theoretically designed HIV-1 non-nucleoside reverse transcriptase inhibitors derived from nevirapine", J. Mol. Model, 20(10), 2450 (2014).

264. Tong Zhu, John Z. H. Zhang and Xiao He, "Correction of erroneously packed protein's side chains in the NMR structure based on ab initio chemical shift calculation" Phys. Chem. Chem. Phys. 16(34), 18163-18169 (2014).

265. Xiao He, Tong Zhu, Xianwei Wang, JInfeng Liu, and John Z. H. Zhang, "Fragment quantum mechanical calculation of proteins and its applications" Acc. Chem. Res.47(9) 2748-2757 (2014).

266. Jiali Gao, John Z. H. Zhang, Kendall N Houk, "Beyond QM/MM: Fragment quantum mechanical methods" Acc. Chem. Res. 47(9), 2711-2711 (2014).

267. Lirong Mou; Xiangyu Jia; Ya Gao; Yongxiu Li; Zhang J.Z.H; Ye Mei, "Folding simulation of Trp-cage utilizing a new AMBER comatible force field with coupled main chain torsion" J. Theor. Comput. Chem., 13. 1450026 (2014).

268. Kunzhong Song; Ju Bao; Yueming Sun; Zhang, J.Z.H., “Binding of N-substituted pyrrole derivatives to HIV-1 gp41”, J. Theor.Comput. Chem., 13(2):1450018 (2014).

269. Duan, L.L.; Ye Mei; Zhang, Q.G.; Bo Tang; Zhang, J.Z.H., “Protein's native structure is dynamically stabilized by electronic polarization”, J. Theor. Comput. Chem.,13, 1440005 (2014).

270. Zhang, Lujia; Gao, Bei; Yuan, Zuanning; He, Xiao; Yuan, Y Adam; Zhang, John Z H; Wei, Dongzhi, “Structure, mechanism, and enantioselectivity shifting of lipase LipK107 with a simple way”, Biochimica et biophysica acta,1844(7):1183-92 (2014).

271. Duan LL, Zhu T, Zhang QG, Tang B, Zhang JZH., “Electronic polarization stabilizes tertiary structure prediction of HP-36”, J. Mol. Model., 20(4):2195 (2014).

272. Lin B. B.; Gao Y.; Li Y. X; Zhang J. Z. H.; Mei Y., “Implementing electrostatic polarization cannot fill the gap between experimental and theoretical measurements for the ultrafast fluorescence decay of Myoglobin”, J. Mol. Model., 20, 2189 (2014).

273. Jia, Xiangyu; Zeng, Juan; Zhang, John Z. H.; et al. “Accessing the Applicability of Polarized Protein-Specific Charge in Linear Interaction Energy Analysis", J. Comput. Chem. 35(9): 737-749 (2014).

274. Song, Jianing; Ji, Changge; Zhang, John Z. H., “Insights on Na+ binding and conformational dynamics in multidrug and toxic compound extrusion transporter NorM”, Proteins: Structure, Function, and Bioinformatics. 82(2): 240-249 (2014).

275. Ji, Chang G.; Mei, Ye; Zhang, John Z. H., “Protein structure and dynamics-polarization in MD simulation”, Abstr. Am. Chem. Soc. 248 (2014).

276. Min Li; John Z.H. Zhang; Fei Xia, "Heterogeneous elastic network model improves description of slow motions of proteins in solution", Chem. Phys. Lett. 618(2), 102 (2015).

277. Zhu, Tong; Zhang, John Z. H.; He, Xiao, “Quantum Calculation of Protein NMR Chemical Shifts Based on the Automated Fragmentation Method”, Adv. Exp. Med. Biol. 827: 49-70 (2015).

278. Zhu, Tong; He, Xiao; Zhang, John Z. H.,” Fragment density functional theory calculation of NMR chemical shifts for proteins with implicit solvation” Phys. Chem. Chem. Phys.,17,18:12367-12367 (2015).

279. Song, Jianing; Li, Yongle; Ji, Changge; Zhang, John Z. H., “Functional Loop Dynamics of the Streptavidin-Biotin Complex”, Sci. Rep., 5, 7906 (2015).

280. Li, Yongxiu; Zhang, John Z. H.; Mei, Ye, “Molecular Dynamics Simulation of Protein Crystal with Polarized Protein-Specific Charge”, Biophys. J., 108, 2: 160A-160A (2015).

281. Gao, Ya; Li, Yongxiu; Zhang, JZH; Mei, Ye, “A Coupled Two-Dimensional Main Chain Torsional Potential for Protein Dynamics”, Biophys. J., 108, 2:159A-160A (2015).

282. Gao, Ya; Li, Yongxiu; Mou, Lirong; Hu, Wenxin; Zheng, J; Zhang, JZH; Mei, Y, “Coupled Two-Dimensional Main-Chain Torsional Potential for Protein Dynamics II: Performance and Validation”, J. Phys. Chem. B, 119,11: 4188-4193(2015).

283. Gao, Ya; Li, Yongxiu; Mou, Lirong; Lin, BB; Zhang, JZH; Mei, Y, “Correct folding of an alpha-helix and a beta-hairpin using a polarized 2D torsional potential”, Sci. Rep.,5 ,10359 (2015).

284. Wang, Xingyu; Ji, Chang G.; Zhang, John Z. H., “Glycosylation Modulates Human CD2-CD58 Adhesion via Conformational Adjustment”, J. Phys. Chem. B, 119, 22: 6493-6501(2015).

285. Yang, Junru; Song, Jianing; Zhang, JZH; Ji, CG, “Effect of mismatch on binding of ADAR2/GluR-2 pre-mRNA complex”, J. Mol. Model., 21, 9(2015).

286. Chen, JZ; Wang, XY; Zhu, T; Zhang, QG; Zhang, JZH, “A Comparative Insight into

Amprenavir Resistance of Mutations V32I, G48V, I50V, I54V, and I84V in HIV-1 Protease Based on Thermodynamic Integration and MM-PBSA Methods", J. Chem. Inf. Model., 55 ,9: 1903-1913(2015).

287. Wang, Xianwei; Zhang, John Z. H.; He, Xiao, "Quantum mechanical calculation of electric fields and vibrational Stark shifts at active site of human aldose reductase", J. Chem. Phys., 143, 18, 184111(2015).

288. Xiangyu Jia, Ye Mei, John Z.H. Zhang, Yan Mo, "Hybrid QM/MM study of FMO complex with polarized proteinspecific charge", Sci. Rep., 5,17096(2015).

289. Jinfeng Liu, Tong Zhu, Xianwei Wang, Xiao He and John Z. H. Zhang, "Quantum Fragment Based ab Initio Molecular Dynamics for Proteins", J. Chem. Theory Comput. 11, 5897−5905 (2015).

290. Jinfeng Liu, Xianwei Wang, John Z. H. Zhang and Xiao He, "Calculation of protein–ligand binding affinities based on a fragment quantum mechanical method", RSC Adv., 5, 107020(2015).

291. J.F. Liu, J.Z.H. Zhang, X. He, "Fragment quantum chemical approach to geometry optimization and vibrational spectrum calculation of proteins", Phys. Chem. Chem. Phys., 18, 1864-1875 (2016).

292. X.Y. Jia, M.T. Wang, Y.H. Shao, G. König, B.R. Brooks, J.Z.H. Zhang, Y. Mei, "Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics", J. Chem. Theory Comput., 12, 499–511 (2016).

293. M. Li, J.Z.H. Zhang, F. Xia, "A new algorithm for construction of coarse-grained sites of large biomolecules", J. Comput. Chem., 37, 795–804 (2016).

294. X. Liu, J.F. Liu, T. Zhu, L.J. Zhang, X. He, and J.Z.H. Zhang, "PBSA_E: A PBSA-Based Free Energy Estimator for Protein–Ligand Binding Affinity", J. Chem. Inf. Model., 56, 854-861 (2016).

295. L.L. Duan, X. Liu, J.Z.H. Zhang, "Interaction Entropy: A New Paradigm for Highly Efficient and Reliable Computation of Protein–Ligand Binding Free Energy", J. Am. Chem. Soc., 138, 5722–5728 (2016).

296. Y. Liu, Z.Z. Yu, J.Z.H. Zhang, L. Liu, F. Xia, J.L. Zhang, "Origins of unique gold-catalysed chemo-and site-selective C–H functionalization of phenols with diazo compounds", Chem. Sci., 7, 1988-1995 (2016).

297. Y. Liu, Z.Z. Yu, Z.J. Luo, J.Z.H. Zhang, L. Liu, F. Xia, "Mechanistic Investigation of Aromatic C (sp2)–H and Alkyl C (sp3)–H Bond Insertion by Gold Carbenes", J. Phys. Chem. A, 120(11), 1925-1932 (2016).

298. M. Li, J.Z.H. Zhang, F. Xia, "Constructing Optimal Coarse-Grained Sites of Huge Biomolecules by Fluctuation Maximization", J. Chem. Theory Comput., 12(4), 2091-2100 (2016).

299. X.W. Wang, X. He, J.Z.H. Zhang, "Accurate Calculation of Electric Fields Inside Enzymes",

Methods in Enzymology, 578, 45-72 (2016).

300. Y. Wang, J.F. Liu, T. Zhu, L.J. Zhang, X. He, J.Z.H. Zhang, "Predicted PAR1 inhibitors from multiple computational methods", Chem. Phys. Lett., 659, 295-303 (2016).

301. M. Li, F.J. Liu, J.Z.H. Zhang, "TMFF-A Two-Bead Multipole Force Field for Coarse-Grained Molecular Dynamics Simulation of Protein", J. Chem. Theory Comput. 12, 6147-6156 (2016).

302. F.J. Liu, J.Z.H. Zhang, Y. Mei, "The origin of the cooperativity in the streptavidin-biotin system: A computational investigation through molecular dynamics simulations", Sci. Rep., 6, 27190 (2016).

303. Y.X. Li, S.Q. Zhang, J.Z.H. Zhang, X. He, "Assessing the performance of popular QM methods for calculation of conformational energies of trialanine", Chem. Phys. Lett., 652, 136-141 (2016).

304. Z.Q. Yao, L.J. Zhang, B. Gao, D.B. Cui, F.Q. Wang, X. He, J.Z.H. Zhang, D.Z. Wei, "A Semiautomated Structure-Based Method to Predict Substrates of Enzymes via Molecular Docking: A Case Study with Candida antarctica Lipase B", J. Chem. Inf. Model., 56, 1979-1994 (2016).

305. J. Zeng, Y.X. Li, J.Z.H. Zhang, Y. Mei, "Examination of the quality of various force fields and solvation models for the equilibrium simulations of GA88 and GB88", J. Mol. Model., 22, 177 (2016).

306. B. Peng, X.Y. Ding, C. Sun, W. Liu, J.Z.H. Zhang, X. Zhao, "The effect of POPC acyl chains packing by aromatic amino acid methyl esters investigated by ATR-FTIR combined with QM calculations", RSC Adv., 6, 45569-45577 (2016).

307. Y. Liu, Z.J. Luo, J.Z.H. Zhang, F. Xia, "DFT Calculations on the Mechanism of Transition-Metal-Catalyzed Reaction of Diazo Compounds with Phenols: O-H Insertion versus C-H Insertion", J. Phys. Chem. A, 120, 6485-6492 (2016).

308. J.F. Liu, Y.Q. Wang, Z.H. Zhang, X. He, "Quantum mechanical mechanism of binding of 4‐anilinoquinazoline inhibitors to the epidermal growth factor receptor based on MFCC computation", China Sciencepaper, 11(18), 2050-2056 (2016).

309. X.S. Jin, T. Zhu, J.Z.H. Zhang, X. He, "A systematic study on RNA NMR chemical shift calculation based on the automated fragmentation QM/MM approach", RSC Adv., 6, 108590-108602 (2016).

310. Z.X. Sun, X.H. Wang and John Z. H. Zhang, "BAR-based optimum adaptive sampling regime for variance minimization in alchemical transformation", Phys.Chem.Chem.Phys.,19, 15005 (2017).

311. Y. Wang, J.F. Liu, L.J. Zhang, X. He, John Z.H. Zhang, "Computational search for aflatoxin binding proteins", Chem. Phys. Lett., 685, 1-8 (2017).

312. L.L. Duan, T. Zhu, C.G. Ji, Q.G. Zhang, John Z.H. Zhang, "Direct folding simulation of helical proteins using an effective polarizable bond force field", Phys. Chem. Chem. Phys.,

19(23), 15273-15284 (2017).

313. L.L. Duan, T. Zhu, Y.C. Li, Q.G. Zhang, John Z.H. Zhang, “Effect of polarization on HIV-1protease and fluoro-substituted inhibitors binding energies by large scale molecular dynamics simulations”, Sci. Rep., 7, 42223 (2017).

314. J.F. Liu, L.W. Qi, John Z.H. Zhang, X. He, “Fragment Quantum Mechanical Method for Large-Sized Ion-Water Clusters”, J. Chem. Theory. Comput. 13(5), 2021-2034 (2017).

315. X.S. Jin, John Z.H. Zhang, X. He, “Full QM Calculation of RNA Energy Using Electrostatically Embedded Generalized Molecular Fractionation with Conjugate Caps Method”, J. Phys. Chem. A, 121(12), 2503-2514 (2017).

316. Y.N. Yan, M.Y. Yang, C.G. Ji, John Z.H. Zhang, “Interaction Entropy for Computational Alanine Scanning”, J. Chem. Inf. Model., 57(5), 1112-1122 (2017).

317. M. Li, John Z.H. Zhang, “Protein simulation using coarse-grained two-bead multipole force field with polarizable water models”, J. Chem. Phys., 146(6), 065101 (2017).

318. Y.N. Yan, W.J. Wang, Z.X. Sun, John Z.H. Zhang, C.G. Ji, “Protein-Ligand Empirical Interaction Components for Virtual Screening”, J. Chem. Inf. Model., 57(8), 1793-1806 (2017).

319. J.F. Liu, X. He, John Z.H. Zhang, “Structure of liquid water - a dynamical mixture of tetrahedral and 'ring-and-chain' like structures”, Phys. Chem. Chem. Phys., 19(19), 11931-11936 (2017).

320. M. Li, John Z.H. Zhang, “Two-bead polarizable water models combined with a two-bead multipole force field (TMFF) for coarse-grained simulation of proteins”, Phys. Chem. Chem. Phys., 19(10), 7410-7419 (2017).

321. Z.X. Sun, Y.N. Yan, M.Y. Yang, John Z.H. Zhang, “Interaction entropy for protein-protein binding”, J. Chem. Phys., 146, 124124 (2017).

322. Z.X. Sun, T. Zhu, X.H. Wang, Y. Mei, John Z.H. Zhang, “Optimization of convergence criteria for fragmentation methods”, Chem. Phys. Lett., 687, 163-170 (2017).

323. Z.X. Sun, X.H. Wang, John Z.H. Zhang, “Protonation-dependent base flipping in the catalytic triad of a small RNA”, Chem. Phys. Lett., 684, 239-244 (2017).

324. M.M. Huang, Z.J. Luo, T. Zhu, J. Chen, John Z.H. Zhang, F. Xia, “A theoretical study of the substituent effect on reactions of amines, carbon dioxide and ethylene oxide catalyzed by binary ionic liquids”, RSC Adv., 7(81), 51521-51527 (2017).

325. L. Liu, F. Zhao, W. Liu, T. Zhu, John Z.H. Zhang, C. Chen, Z.H. Dai, H.S. Peng, J.L. Huang, Q. Hu, W.B. Bu, and Y. Tian, “An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O2 in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy”, Angew. Chem.-Int. Edit., 56, 35, 10471-10475 (2017).

326. S. Li, A.W. Zhu, T. Zhu, John Z.H. Zhang, and Y. Tian, “Single Biosensor for Simultaneous

Quantification of Glucose and pH in a Rat Brain of Diabetic Model Using Both Current and Potential Outputs", Anal. Chem., 89, 6656−6662 (2017).

327. Y. Gao, C.M. Zhang, John Z.H. Zhang, and Y. Mei, "Evaluation of the Coupled Two-Dimensional Main Chain Torsional Potential in Modeling Intrinsically Disordered Proteins", J. Chem. Inf. Model., 57, 267−274 (2017).

328. L.Q. Qiu, Y.N. Yan, Z.X. Sun, J.N. Song, John Z.H. Zhang, "Interaction entropy for computational alanine scanning in protein–protein binding", WIREs Comput. Mol. Sci., doi: 10.1002/wcms.1342 (2017).

329. Sun, HY; Duan, L; Chen, F; Liu, H; Wang, Z; Pan, PC; Zhu, F; Zhang, JZH; Hou, TJ, "Assessing the performance of MM/PBSA and MM/GBSA methods. 7. Entropy effects on the performance of end-point binding free energy calculation approaches", Phys. Chem. Chem. Phys. 20, 14450-14460 (2018)

330. Xu, Mingyuan; Zhu, Tong; Zhang, John Z. H. "A Force Balanced Fragmentation Method for ab Initio Molecular Dynamic Simulation of Protein", FRONTIERS IN CHEMISTRY, 6, 189 (2018).

331. Jin, Xinsheng; Zhu, Tong; Zhang, John Z. H.; et al. "Automated Fragmentation QM/MM Calculation of NMR Chemical Shifts for Protein-Ligand Complexes", FRONTIERS IN CHEMISTRY, 6, 150 (2018).

332. Wang, Jingxue; Cao, Huali; Zhang, John Z. H.; et al. "Computational Protein Design with Deep Learning Neural Networks", SCIENTIFIC REPORTS, 8, 6349 (2018).

333. Liu, Xiao; Peng, Long; Zhou, Yifan, Zhang, Youzhi, Zhang, John Z.H., "Computational Alanine Scanning with Interaction Entropy for Protein-Ligand Binding Free Energies", J. Chem. Theory Comput. 14, 1772-1780 (2018).

334. Qiu, Linqiong; Yan, Yuna; Sun, Zhaoxi, Song, Jianing, Zhang, John Z.H., "Interaction entropy for computational alanine scanning in protein-protein binding",

335. WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE, 8, e1342 (2018)

336. Liu, Jinfeng; He, Xiao; Zhang, John Z. H.; et al. "Hydrogen-bond structure dynamics in bulk water: insights from ab initio simulations with coupled cluster theory". Chem. Sci. 9, 2065-2073 (2018).

337. Liu, Jinfeng; Swails, Jason; Zhang, John Z. H.; et al. "A Coupled Ionization-Conformational Equilibrium Is Required To Understand the Properties of Ionizable Residues in the Hydrophobic Interior of Staphylococcal Nuclease", J. Am. Chem. Soc. 140, 1639-1648 (2018).

338. Wang, Xiaohui; Tu, Xingzhao; Zhang, John Z. H.; et al. BAR-based optimum adaptive sampling regime for variance minimization in alchemical transformation: the nonequilibrium stratification", Phys. Chem. Chem. Phys. 20, 2009-2021 (2018).

339. Song, Jianing; Qiu, Linqiong; Zhang, John Z. H. “An efficient method for computing excess free energy of liquid”, Sci. Chi. Chem., 61, 135-140 (2018).