张增辉

John Z.H. Zhang

1. 联系方式

E-mail: john.zhang@nyu.edu，**zh.zhang1@siat.ac.cn**
Tel : +86 21 2059 6018

2. 教育和工作经历

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-	华东师范大学国家特聘教授
2013-	NYU global network professor，Director of NYU-ECNU Center for Computational Chemistry
2021-	讲习教授，中国科学院深圳理工大学合成生物学院（筹）/深圳先进技术研究院合成生物所

3. 专业服务

Journal Editorship

1998-2002	*Theoretical Chemistry Accounts*, Advisor editor
2001-2008	*Journal of Theoretical and Computational Chemistry*, Editor-in-Chief
2008-12	*Science in China B-Chemistry*, Editorial board
2015-2018	*Scientific Reports*, Editorial board
2015-2018	*Chemical Physics Letters*, Editor
2008-	*Journal of Computational Biophysics and Chemistry*, Advisory editor
2002-	*Chinese Journal of Chemical Physics*, Editorial board
2017-	*Frontiers in Biomolecular Science*, Associate Editor
2018-	*Computational and Mathematical Biophysics*, Editorial board
2019-	*Physical Chemistry Chemical Physics*, Associate Editor
2020-	*Molecules*, Editorial board
2021-	*J. Chemical Information and Modeling*, Editorial board

Professional Society

2010-	中国化学会理论与计算化学专业委员会委员

2010- 中国生物化学和分子生物学会蛋白质专业委员会委员

2010- 大连化物所分子反应动力学国家重点实验室学术委员会委员

2020-2023 宁波大学新药技术研究院第一届学术委员会委员

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
2000 基金委海外杰出青年基金（B 类）
2003 第五批长江特聘讲座教授
2009 首批国家特聘教授
2016 第六届中国侨界贡献奖
2021 Fellow of the Royal Society of Chemistry (United Kingdom)

5. 主要学术贡献

张增辉早期发展了几何变分方法和含时波包方法，成功解决了多原子体系的量子反应动力学的精确数值计算问题，在国际化学反应动力学领域做出了原创性的贡献，撰写的专著《Theory and Application of Quantum Reaction Dynamics》（World Scientific, 1998） 是化学反应动力学领域的权威参考书；2013 年发展了原创性的碎片共轭线性标度量子计算方法（MFCC）来研究大分子的相互作用以及蛋白在溶液中的性质，该方法的创新性和有效性获得了国际同行的高度评价，被 Chem. Rev.专题文章进行重点介绍，是目前国际上研究大分子体系的量子分块理论计算方法的重要基础；2008 年发展了基于精确量子化学计算的蛋白质静电极化专一性电荷（PPC）方法，广泛用于蛋白质结构和动力学、蛋白-配体复合体结构性质研究和自由能计算；2016 年发展了相互 作用熵方法用于高效计算蛋白-配体相互作用自由能中的熵变，避免了耗费计算时间的正则振动模式的计算。

6. 目前主要研究方向：

基于计算生物方法和人工智能技术研究生物分子体系的性质与功能，包括蛋白质的结构与功能，药物分子和蛋白的设计，酶催化反应的计算模拟，定量进化的数字化模拟等。

7. Citations of Publications

Number of Publications: >400
Number of times cited: >12,000 (web of science)
h-index: 59 (web of science), 67 (google scholar)

2019 年 Elsevier 中国高被引学者（化学）https://www.elsevier.com/zh-cn/solutions/scopus/most-cited/chemistry-2019

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. LEEHUANG S; LIN H P; ZHANG D; ZHANG J Z H; CHANG Y T; LEE J W; BAO J; SUN Y; HUANG P L, "Compositions and methods for treating obesity, obesity related disorders and for inhibiting the infectivity of human immunodeficiency virus", US9132145-B2, September. 15, 2015.

4. 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, November 5, 2013

5. 何晓，刘金峰，张增辉， "一种非核苷类HIV-1反转录酶抑制剂", 专利号201310242563.7，Nov. 18, 2015

6. 季长鸽，闫玉娜，张增辉，"基于相互作用指纹和机器学习的药物靶标的虚拟筛选方法"，专利号： 201610852817.0， Nov. 9, 2018.

7. 潘月，张鲁嘉，张增辉，何晓，张传玺，方波欢，"一种基于酵母二肽基肽酶III的抗体模拟物及其应用"，专利号：ZL 202010192357.X， 2020年10月20。

8. 赵玥，张鲁嘉，张增辉，何晓，方波欢，"一种基于α螺旋融合两种蛋白质且保持各自亚基活性的蛋白质融合设计方法"，专利号：202010192367.3, 2020年3月18。

9. 赵玥，张鲁嘉，张增辉，韩艳芳，何晓，方波欢，"一种表达微管β亚基与蛋白A的D结构域融合蛋白的基因工程菌株及其构建方法"，专利号：202010207523.9，2020年3月23。

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 → 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 (coorganizer).

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).

128. NYUSH Symposium on Chemical Biology, Shanghai, China, March 12-13, 2018 (organizer and speaker)

129. Shanghai Eastern Forum, Shanghai, China , May 2-4, 2018 (invited speaker)

130. Workshop on Mathematics of Drug Design/Discovery, Toronto, Canada, June 3-7, 2018, (invited speaker).

131. The 2nd Worldwide Chinese Computational Biology and Molecular Simulation,

Guangzhou, China, June 7-10, 2018 (Chairman and speaker）

132. Computational Chemical Dynamics: A Symposium in Honor of Donald J. Kouri , Shanghai, China, June 12, 2018 (organizer and speaker)

133. First Conference of Theoretical and Computational Chemistry at Beijing National Research Center for Molecular Sciences, , Beijing, China, August 4-6, 2018 (invited speaker).

134. The Second JiaXiu Workshop, Guiyang, China, August 8-11, 2018 (plenary speaker)

135. The 3rd QiLu Young Scientists' Forum, Qingdao, China, October 16-18，2018 (invited speaker).

136. International Conference on Theoretical and High Performance Computational Chemistry, Tianjin, China, October, 19-22, 2018 (invited speaker).

137. International Workshop on Milliseconds Simulation for Millions Atoms within 100 Days, Dalian, China, October 26-29 2018 (invited speaker).

138. Application of CADD and AI in New Drug Development， Shanghai, China， November 4, 2018 (Keynote speaker).

139. 12/10-14, "Computational and Mathematical Approaches for Bioinformatics and Biophysics" (TSIMF), Sanya, China，December 10-14, 2018 (invited speaker).

140. Development and application potential of machine learning methods in drug discovery, protein design and synthetic biology, The 237th NSFC Shuangqing Symposium, "Chinese chemistry in the age of AI", Shenzhen, China, Mary 24-27, 2019. (Invited speaker)

141. Computational Study of Protein Structure and Dynamics from Force Field to Ab Initio, Belgrade Workshop, Institut za Nuklerne Nauke "VINCA", Belgrade, Serbia, July 26-28, 2019 (Plenary speaker)

142. Free energies in protein-protein and protein-ligand bindings, The 14th Femto-chemistry Conference: Dynamics of the Complexity in Chemistry, Shanghai, China, July 28-Aug. 2, 2019 (Plenary speaker)

143. Free energies in protein-protein and protein-ligand bindings, Summer workshop & school, "Computational Biology: from molecules to systems", Dongguan, China, July 31-Aug. 4, 2019 (Plenary speaker)

144. Theory and Simulation of Biomolecules: Present and Future, Strategic Symposium in Modern Theoretical Chemistry, Tianshui, China, Aug. 3-7, 2019 (Plenary speaker)

145. Methods for Free Energy Analysis In Protein-Protein Interaction, Symposium on Statistical Mechanics of Complex Systems, Nanjing, China, Nov. 9-12, 2019 (Plenary speaker)

146. Free energy analysis in protein-substrate binding, "Symposium on from Free Energy

Perturbation Theory to Biomedicine: The link Between Theory and Life. Shenzhen, China, Nov. 9-12, 2019 (Invited speaker)

147. Free Energy Analysis in Protein-Substrate Binding, The 15th National Congress of Computational Chemistry of the Chinese Chemical Society, Shanghai, Nov. 14-17, 2019 (Plenary speaker)

148. Free Energy Analysis in Protein-Ligand Binding, The 8th Cross Strait Conference on Theoretical and Computational Chemistry, Taipei, Taiwan, Dec. 5-9, 2019 (Invited speaker)

149. Study of Protein-Protein Interaction, The 2nd Conference on Computational and Mathematical Bioinformatics and Biophysics, Sanya, China, Dec. 10-15, 2019 (Invited speaker).

150. Free Energy Analysis of Protein Interaction, "The 3rd Worldwide Chinese Conference of Computational Biology", Beijing, China, August 3-6，2020 (Invited speaker).

151. Computational Study of Protein Interaction, "Conference Commemorating Prof. Chonghao Deng's 100th Birthday", Jinan, China, October 10-11, 2020 (invited speaker).

152. Frontier Symposium in Theoretical and Computational Chemistry, Nanjing, China, October 24-26，2020 (Session chair).

153. Free Energy Analysis of Protein Interaction, Seminar, Shanghai Jiaotong University, Nov. 25, 2020.

154. International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry, Shenzeng, China, December 4-7, 2020, (invited speaker).

155. Development and Application of computational Methods for Protein Interaction and Drug Design, Seminar, Seminar, Byte Dance AI Lab, Shanghai, Dec. 29.

156. "Conference on Computational Statistical Mechanics of Complex Systems", Hangzhou, China, December 12-13, 2020 (Session Chair).

157. 蛋白-配体相互作用的微观机制, Seminar, Sichuan University, March 23, 2021.

158. Simulation of Complex Chemical Reactions, "ACS Spring 2021 Symposium in honor of Donald J. Kouri", April 5-8, 2021 (invited speaker).

159. "生物分子的设计与计算方法研究"，第七届全国计算生物学与生物信息学学术会议（NCCBB）暨国际人工智能与生物医学信息大会（ICAIPMI），July 16-18，Yantai （invited speaker）。

160. 前沿生物技术探索与科研伦理治理探讨"，生命科学与科研伦理道德"科学与治理战略研讨会（深圳），Sept. 24. (Invited speaker).

161. 白与配体相互作用结构与自由能计算研究， 北京香山会议，北京，Sept. 29-30, 2021 (invited speaker).

162. 蛋白-配体互作复合物的结构预测与自由能计算, 第十四届全国量子化学大会，上海，Oct. 9-12，2021 （invited speaker）。

163. 蛋白-配体互作复合物的结构预测与自由能计算, 第十六届全国计算（机）化学大会，长春，Oct. 18-20，2021 （Keynote speaker）。

164. 世界顶尖科学家会议, 上海，Oct. 31，2021 (主题演讲和圆桌论坛)。

165. "Structure and interaction of protein-ligand complex", The Fourth TSIMF Conference on Computational and Mathematical Bioinformatics and Biophysics, Virtual Conference，Dec. 13-16, 2021 (invited speaker).

List of Research Publications:

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