John Z.H. Zhang

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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

2019-	Physical Chemistry Chemical Physics, **Associate Editor**
2018-	*Molecular Based Mathematical Biology,* Editorial board
2015-	*Scientific Reports*, Editorial board
2015-	*Frontiers in Molecular Biosciences,* Associate Editor
2015-	*Interdisciplinary Sciences: Computational Life Sciences*, Editorial board
2008-	*Journal of Theoretical and Computational Chemistry,* Advisory editor
2002-	*Chinese Journal of Chemical Physics,* Editorial board

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. **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.

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

7. **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).

Recent Research Publications:

1. 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).

2. 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).

3. 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).

4. 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).

5. 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).

6. 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).

7. 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).

8. 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).

9. X.W. Wang, X. He, J.Z.H. Zhang, “Accurate Calculation of Electric Fields Inside Enzymes”, Methods in Enzymology, 578, 45-72 (2016).

10. 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).

11. 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).

12. 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).

13. 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).

14. 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).

15. 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).

16. 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).

17. 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).

18. 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).

19. 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).

20. 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).

21. 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).

22. 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).

23. 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).

24. 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).

25. 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).

26. 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).

27. 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).

28. 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).

29. 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).

30. 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).

31. 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).

32. 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).

33. 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).

34. 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).

35. 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).

36. 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).

37. 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).

38. 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).

39. 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)

40. 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).

41. 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).

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

43. 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).

44. Qiu, Linqiong; Yan, Yuna; Sun, Zhaoxi, Song, Jianing, Zhang, John Z.H., “Interaction entropy for computational alanine scanning in protein-protein binding”, "Wiley Interdiscip Rev. Comput. Mol. Sci.”, 8, e1342 (2018)

45. 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).

46. 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).

47. 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).

48. 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).