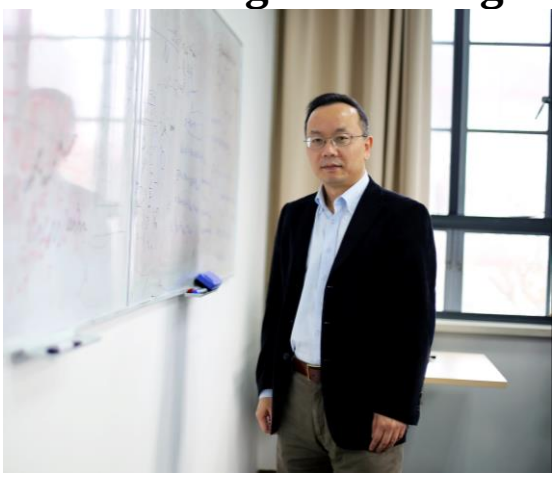
John Zeng Hui Zhang



1. **Contact Address**

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Department of Physics, College of Chemistry and Molecular Engineering, East China Normal University, Shanghai, China

Department of Chemistry, New York University

2. Education and Professional Experience

1978-1987	East China Normal University, BA
1982-1987	University of Houston, Ph. D in Physics
1987-1990	UC Berkeley, Postdoctoral Fellow，Assistant Researcher
1990-1994	Dept. of Chemistry, New York University, Assistant Professor
1994-1997	Dept. of Chemistry, New York University, Associate Professor
1997	Hong Kong University of Science & Technology, Visiting Professor
1997-2001	Dept. of Chemistry, New York University, Associate Professor National University of Singapore, Visiting Professor
2001-2008	Nanjing University，Director of Institute of Theoretical & Computational Science
2003-2008	Nanjing University, Changjiang Lecture Professor
2005	Institute of Atomic and Molecular Science, Taiwan, Visiting Professor
2013-	Professor, NYU Shanghai

3. Professional Service

1998-2002	*Theoretical Chemistry Accounts,* Advisor editor
2008-	*Journal of Theoretical and Computational Chemistry,* Advisory Editor
2002-	*Chinese Journal of Chemical Physics,* Advisor editor
2008-12	*Science in China B-Chemistry,* Advisor editor

2015- *Scientific Reports*, Advisor Editor
2015- *Chemical Physics Letters*, Editor

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, Chinese Academy of Science
2001	NSFC Outstanding Overseas Young Scientist Award
2003	Changjiang Lecture Professorship
2009	"Thousand Talent Program"

5. Current Research Area：Theoretical and Computational Chemistry & Biology

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, etc.

6. 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).

7. 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

8. Citations of Research Publications

No. of times cited:	**8800**
h-index**:**	**50**

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 + 2 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).

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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).

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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).

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

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

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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).

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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).

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