

# 个人简历

## 基本信息

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专业: 物理化学      毕业院校: 香港科技大学      最高学历: 博士      政治面貌: 中共党员  
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## 教育/工作背景

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2016.04 - 至今	中国科学技术大学	化学物理系	副研究员
2014.09 - 2016.03	香港科技大学	化学系	博士后 (导师: 严以京)
2010.09 - 2014.08	香港科技大学	纳米科技研究所	博士 (导师: 严以京)
2006.09 - 2010.07	中国科学技术大学	化学物理系	本科 (导师: 徐瑞雪)

## 研究方向

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- 复杂系统动力学理论和方法
- 凝聚相超快分子动力学和化学反应机理
- 光合系统和光伏材料中能量传递、电荷转移和分离过程
- 纳米器件中的量子输运、量子测量和量子调控
- 量子统计、量子热力学理论和应用

## 基金项目

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|-----------------|-----------|--------|
| • 国家自然科学基金青年项目  | 2018-2020 | 主持, 在研 |
| • 安徽省自然科学基金青年项目 | 2017-2019 | 主持, 在研 |
| • 青年创新基金        | 2017-2018 | 主持, 在研 |
| • 科技部重大专项       | 2016-2021 | 参加, 在研 |

## 科研成果

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1. 系统的发展了非微扰、非马尔科夫的量子耗散理论, 解决了一系列复杂体系的量子动力学问题
2. 开发了一套精确、高效的开放量子系统计算程序包[[OpenQuant](#)], 结合分子动力学和量子化学计算, 应用到超快分子动力学、化学反应机理、量子生物过程等研究领域
3. 结合非线性光谱模拟和速率计算, 揭示了光合体系中长时间量子震荡的成因以及量子相干促进能量传递的微观机理
4. 研究了一系列受环境和外场调制的 Fano 共振动力学, 为发展分子原子器件和生物传感技术提供理论支持

## 教学科研技能

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- 在基础理论知识方面有扎实的基本功，本科和博士所修专业课程均取得优异成绩，包括：物理化学、量子化学、统计力学、分子反应动力学、分子光谱等
- 可以独立完成自然科学课题的研究工作并发表在国际主流学术期刊
- 有扎实的算法功底和编程基础，在大型线性系统求解、聚类分析、并行计算等方面有丰富的经验，熟练使用 C/C++/Fortran/Python/Mathematica/Matlab/Bash/Cuda 等科学计算和脚本语言
- 具备多年 Linux 集群的管理和维护经验，包括系统、软件环境的安装和部署等
- 与美国韦恩州立大学的 Vladimir Chernyak 教授、香港科技大学的黄旭辉教授、中科大的严以京、郑晓教授等国内外优秀科研团队有密切的合作关系

## 发表论文

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期刊论文:

1. **H. D. Zhang\***, Y. J. Yan\*, and V. Chernyak\*, How to probe coherent energy transfer with quantum single-molecule measurement: Response theory without driving field, *J. Phys. Chem. Lett. in preparation*.
2. **H. D. Zhang\***, Y. J. Yan\*, and V. Chernyak\*, Coherent energy transfer probed by single-molecule measurements and quantum measurement theory, *J. Chem. Phys. to be submitted*.
3. **H. D. Zhang\***, H. Gong, R. X. Xu, X. Zheng\*, and Y. J. Yan, Thermodynamics of open quantum systems: A linear response perspective, *J. Chem. Phys. Comm. to be submitted*
4. L. Cui, **H. D. Zhang\***, X. Zheng\*, R. X. Xu, and Y. J. Yan, Highly efficient and accurate sum-over-poles expansion of Fermi and Bose functions at near zero temperatures: Fano spectrum decomposition scheme, *J. Chem. Phys. submitted*.
5. R. X. Xu\*, X. C. Tao, Y. Wang, Y. Liu, **H. D. Zhang**, Y. J. Yan, A hierarchical-equation-of-motion based semiclassical approach to quantum dissipation, *Chin. J. Chem. Phys.* 31, 608-612 (2018).
6. Y. Wang, Z. J. Pan, **H. D. Zhang\***, and Y. J. Yan\*, Dissipaton dynamics theory versus quantum master equations, *Chem. Phys.* 515, 94-101 (2018, Wolfgang Domcke Festschrift).
7. L. Han, **H. D. Zhang**, X. Zheng\* and Y. J. Yan, On the exact truncation tier of fermionic hierarchical equations of motion, *J. Chem. Phys.* 148, 234108 (2018).
8. Y. Liu, R. X. Xu, **H. D. Zhang**, and Y. J. Yan\*, Dissipaton equation of motion theory versus Fokker-Planck quantum master equation, *Chin. J. Chem. Phys.* 31, 245-256 (2018).
9. P. L. Xu, S. J. Hu, **H. D. Zhang\***, and X. Zheng\*, Theoretical insights into the reactivity of Fe-based catalysts for water oxidation: The role of electron-withdrawing groups, *Phys. Chem. Chem. Phys.* under revision (2018).
10. R. X. Xu, Y. Liu, **H. D. Zhang**, and Y. J. Yan\*, Theories of quantum dissipation and nonlinear coupling bath descriptors, *J. Chem. Phys.* 148, 114103 (2018).
11. **H. D. Zhang\***, R. X. Xu, X. Zheng, and Y. J. Yan\*, Statistical quasi-particle theory for open quantum systems, *Mol. Phys.* 116, 780-812 (2018).
12. R. X. Xu, Y. Liu, **H. D. Zhang**, and Y. J. Yan, Theory of quantum dissipation in a class of non-Gaussian environments, *Chin. J. Chem. Phys.* 30, 395 (2017).

13. Y. Kong, D. Hou, **H. D. Zhang\***, X. Zheng and R. X. Xu, Davydov collective vibrational modes and infrared spectrum features in aniline crystal: Influence of geometry change induced by van der Waals interactions, *J. Phys. Chem. C* 121, 18867-18875 (2017).
14. L. Z. Ye, **H. D. Zhang\***, Y. Wang, X. Zheng and Y. J. Yan, Low-frequency logarithmic discretization of the reservoir spectrum for improving the efficiency of hierarchical equations of motion approach, *J. Chem. Phys.* 147, 074111 (2017).
15. **H. D. Zhang\***, Q. Qiao, R. X. Xu, X. Zheng and Y. J. Yan, Efficient steady-state solver for hierarchical quantum master equations, *J. Chem. Phys.* 147, 044105 (2017).
16. J. J. Ding, Y. Wang, **H. D. Zhang\***, R. X. Xu, X. Zheng and Y. J. Yan, Fokker–Planck quantum master equation for mixed quantum–semiclassical dynamics, *J. Chem. Phys.* 146, 024104 (2017).
17. J. J. Ding, **H. D. Zhang#**, Y. Wang, R. X. Xu, X. Zheng and Y. J. Yan, Minimum–exponents ansatz for molecular dynamics and quantum dissipation, *J. Chem. Phys.* 145, 204110 (2016).
18. **H. D. Zhang\***, Q. Qiao, R. X. Xu and Y. J. Yan, Effects of Herzberg–Teller vibronic coupling on coherent excitation energy transfer, *J. Chem. Phys.* 145, 204109 (2016).
19. **H. D. Zhang**, Q. Qiao, R. X. Xu and Y. J. Yan, Solvent-induced polarization dynamics and coherent two-dimensional spectroscopy: Dissipaton equation of motion approach, *Chem. Phys.* 481, 237-244 (2016).
20. Q. Qiao, **H. D. Zhang** and X. H. Huang, Enhancing pairwise state-transition weights: A new weighting scheme in simulated tempering that can minimize transition time between a pair of conformational states, *J. Chem. Phys.* 144, 154107 (2016).
21. **H. D. Zhang** and Y. J. Yan, Kinetic rate kernels via hierarchical Liouville-space projection operator technique, *J. Phys. Chem. A* 120, 3241-3245, (2016).
22. **H. D. Zhang** and Y. J. Yan, Onsets of hierarchy truncation and self-consistent Born approximation with quantum mechanics prescriptions invariance, *J. Chem. Phys.* 143, 214112 (2015).
23. R. X. Xu, **H. D. Zhang**, X. Zheng, and Y. J. Yan, Dissipaton equation of motion for system-and-bath interference dynamics, *Science China Chemistry* 58, 1816 (2015).
24. Y. Kong, **H. D. Zhang\***, Y. M. Wang, R. X. Xu, and Y. J. Yan, Dissipatons equation of motion with controlled truncation, *Chin. J. Chem. Phys.* 28, 409 (2015).
25. **H. D. Zhang**, R. X. Xu, X. Zheng, and Y. J. Yan, Nonperturbative spin-boson and spin-spin dynamics and nonlinear Fano interferences: A unified dissipaton theory based study, *J. Chem. Phys.* 142, 024112 (2015).
26. J. Xu, **H. D. Zhang**, R. X. Xu, and Y. J. Yan, Correlated driving and dissipation in two-dimensional spectroscopy, *J. Chem. Phys.* 138, 024106 (2013).
27. J. Xu, R. X. Xu, D. Abramavicius, **H. D. Zhang**, and Y. J. Yan, Advancing hierarchical equations of motion for efficient evaluation of coherent two-dimensional spectroscopy, *Chin. J. Chem. Phys.* 24, 497-506 (2011).

图书章节:

1. “Quantum dynamics in dissipative molecular systems”,  
**H. D. Zhang**, J. Xu, R. X. Xu, and Y. J. Yan, in *Advances in Multi-Photon Processes and Spectroscopy: Volume 21, Chapter 5*, pp.177-209, edited by S. H. Lin, A. A. Villaeys, and Y. Fujimura, published by World Scientific, 2013.
2. “Modified Zusman equation for quantum solvation dynamics and rate processes”,

**H. D. Zhang**, J. Xu, R. X. Xu, and Y. J. Yan, in *Reaction Rate Constant Computations: Theories and Applications*, RSC Theoretical and Computational Chemistry Series No. 6, Chapter 13, pp.319-336, edited by Ke-Li Han and Tian-Shu Chu, published by RSC Publishing, 2013.

## 参加学术会议

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2018.12 “2018 Workshop on Comput. and Stat. Mech. of Complex Systems”, Hefei, China  
口头报告: Significance of system-bath entanglement on quantum dynamics and thermodynamics of open systems

2018.09 “Workshop on Quantum Effects in Energy Transfer and Conversion”, Beijing, China  
邀请报告: Coherent energy transfer probed by quantum measurement and response theory

2018.05 “The 31th Annual Conference of Chinese Chemistry Society”, Hangzhou, China

2017.12 “2017 Workshop on Comput. and Stat. Mech. of Complex Systems”, Fuzhou, China  
张贴海报: “Statistical quasi-particle theory for open quantum systems”

2017.06 “The 13th National Conference of Quantum Chemistry”, Dalian, China  
口头报告: “Correlated system-bath dynamics via dissipaton equation of motion approach”

2016.07 “The 30th Annual Conference of Chinese Chemistry Society”, Dalian, China  
口头报告: “Efficient hierarchy truncation with quantum mechanics prescription invariance”

2014.04 “Hong Kong Spring School on Quantum Simulation Methods”, HKU, Hong Kong

2013.10 “2013 International Workshop on Coherence Control”, USTC, Hefei, Anhui, China

2011.07 “Workshop on Photosynthesis Systems”, USTC, Hefei, Anhui, China

2011.05 “The 11th National Conference of Quantum Chemistry”, Hefei, Anhui, China  
张贴海报: “Hierarchical Liouville-space dynamics for multi-dimensional spectroscopy”

2010.12 “Workshop on Simulation and Modeling of Emerging Electronics”, HKU, Hong Kong