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教育经历：

学士： 1995-2000 中国科学技术大学少年班
硕士： 2000-2003 美国罗切斯特大学化学系
博士： 2003-2007 美国加州大学尔湾分校化学系

研究兴趣：

- 发展和建立结合分子动力学模拟、QM/MM构建哈密顿量和格林函数的各类光谱响应的理论框架，用于蛋白质/RNA折叠和误折叠的机理研究。
- 发展对离子溶液中动力学现像及其相关各阶振动光谱进行模拟的理论方法和技术，并与实验结合对溶液及生理环境中离子的影响和特异性进行研究
- 发展用户友好的软件包，在分子动力学计算机模拟和超快实验光谱技术之间搭建桥梁。提供一个独特的方式来验证计算机模拟观测到的物理现象、以及从微观层面解析实验光谱特征。
- 利用超快光谱学研究庞杂的生物体系和生物现象，诸如淀粉样蛋白纤维、生物膜、化学交换、光吸收天线、生物传感及聚合物材料等。

科研经历：

- 2001-2003：美国罗切斯特大学攻读硕士研究生，导师，Prof. **Christoph Dellago**.
  研究内容，*"Transition Path Sampling"*， 一种基于经典和从头算分子动力学模拟的用于小概率事件捕获轨迹系综的高级统计力学方法
- 2003-2007：美国加州大学欧文分校攻读博士研究生，导师Prof. **Shaul Mukamel.**
  研究内容，"SPECTRON" 软件包，该软件包可用于模拟各类复杂体系的相关光谱响应.
- 2007-2009： 美国加州大学伯克利分校做博士后研究员，导师Prof. **David Chandler**
  研究内容，采用统计力学的方法来研究流体固体和气体固体界面上的电子和能量转移过程
- 2010-至今 中科院大连化学物理研究所研究员，博士生导师，课题组组长.

基金项目：

- 国家自然科学基金青年基金（21003117）："紧密结合长程分子动力学计算机模拟和二维红外光谱技术以研究蛋白质折叠的动力学机理"，2011.01-2013.12,21 万元，负责人，已结题
- 国家自然科学基金重点项目（21033008）："光合过程中能量传递的量子动力学理论与模拟"
  2011.01-2014.12,220 万元，主要参与人，在研
- 科技部仪器项目（2011YQ09000505）： "变温碰撞反应飞行时间离子谱测定离子结构应用研

究”2012.01-2017.12 1000 万元，理论计算部分负责人，在研

- 国家自然科学基金面上项目（21373201）：“离子溶液中的微观动力学及其光谱表征理论研究”2014.01-2017.12， 80 万元， 负责人， 在研
- 中科院 B 类先导项目 (XDB10000000)：“页岩气勘探开发基础理论与关键项目”子课题 2014-2018，250 万元， 子课题负责人，在研

发表论文：

1) Ruiting Zhang and Wei Zhuang* ***"****The Effect of Ion Pairing on the Solution Dynamics Investigated by the Simulations of the Optical Kerr Effect and the Dielectric Relaxation Spectra"* **The Journal of Chemical Physics**, **DOI:** 10.1063/1.4863562 (2013)
2) Tianmin Wu, Ruiting Zhang, Huanhuan Li, Lijiang Yang, and Wei Zhuang* *"Discriminating Trpzip2 and Trpzip4 Peptides'Folding Landscape Using the Coherent Vibrational Spectroscopy: a Simulation Study"* **The Journal of Chemical Physics, DOI:** 10.1063/1.4863696 (2013)
3) Qiang Zhang, Ruiting Zhang, Ying Zhao, Huanghuan Li, Yi-Qin Gao, and Wei Zhuang* ***"****Pairing Preferences of the Model Mono-Valence Mono-Atomic Ions Investigated by Molecular Simulation"* **The Journal of Chemical Physics** , (under revision)
4) H.T. Bian，H.L. Chen, Q. Zhang, J.B. Li，X.W. Wen，W. Zhuang* and J.R. Zheng* *"Cation Effects on Rotational Dynamics of Anions and Water Molecules in Alkali (Li+,Na+,K+,Cs+) Thiocyanate(SCN−) Aqueous Solutions"* **J. Phys. Chem. B**, 117 (26), 7972-7984 (2013)
5) Qiang Zhang, Wen Jun Xie, Hongtao Bian, Yi Qin Gao, Junrong Zheng*, and Wei Zhuang* " *Microscopic Origin of the Deviation from Stokes-Einstein Behavior Observed In Dynamics of the KSCN Aqueous Solutions: A MD Simulation Study*" .**J. Phys. Chem. B**, 117 (10), pp 2992–3004 (2013)
6) Tianmin Wu, Lijiang Yang, Ruiting Zhang, Qiang Shao, and Wei Zhuang*. "*Modeling the Thermal Unfolding 2DIR Spectra of a ß Hairpin Peptide Based on the Implicit Solvent MD Simulation*" **J. Phys. Chem. A**, 117,6256−6263 (2013)
7) Ruiting Zhang and Wei Zhuang*."*Effect of Ion Pairing on the Solution Dynamics Investigated by the Simulations of the Optical Kerr Effect and the Dielectric Relaxation Spectra*". **J. Phys. Chem. B**, dx.doi.org/10.1021/jp404923y(2013)
8) Qiang Zhang, Bing-bing Zhang, Ling Jiang* and Wei Zhuang* *"Ion Pairing Kinetics Does not Necessarily Follow the Eigen-Tamm Mechanism"* **Chin. J. Chem. Phys**, 26 (6), 694 (2013)
9) Jian Song, Fang Gao, Raymond Z. Cui, Feng Shuang, Wanzhen Liang, Xuhui Huang, and Wei Zhuang* ."*Investigating the Structural Origin of Trpzip2 Temperature Dependent Unfolding Fluorescence Line Shape Based on a Markov State Model Simulation*". **J. Phys. Chem. B**, 116:12669−12676, (2012)
10) Cyril Falvo*,Wei Zhuang, Yung Sam Kim, Paul H. Axelsen, Robin M. Hochstrasser, and Shaul Mukamel . "*Frequency Distribution of the Amide-I Vibration Sorted by Residues in Amyloid Fibrils Revealed by 2D-IR Measurements and Simulations*". **J. Phys. Chem. B**, 116:3322−3330,(2012)
11) Hongtao Bian, Jiebo Li, Qiang Zhang, Hailong Chen, , Yi Qin Gao*, Junrong Zheng* and Wei Zhuang*. "*Ion Segregation in Aqueous Solutions*". **J. Phys. Chem. B**, 116:14426−14432, (2012)
12) Jian, S., and Wei, Zhuang. "*Coherent Two Dimensional Infrared Spectroscopy of Proteins: Concepts and Simulations*", **Progress in Chemistry** 24, 1065-1081. (2012)
13) Cui, R.Z., Silva, D., Song, J., Bowman, G.R., Zhuang, W*.,Xuhui Huang* "*Bridging the gap between optical spectroscopic experiments and computer simulations for fast protein folding dynamics*", **Curr. Phys. Chem.** 2, 45,(2012)
14) Bian, Hongtao; Wen, Xiewen; Li, Jiebo; Chen Hailong; Han Suzee; Sun Zhigang, Song Jian, W.

Zhuang,, JR Zheng* "*Ion Clustering in Aqueous Solutions Probed with Vibrational Energy Transfer*" **Proceedings of National Academy of Sciences.USA.** 108,4737, (2011) **(highlighted by SCIENCE)**

15) W. Zhuang*; Cui, Raymond; Silva, Daniel-Adriano; Huang, Xuhui "*Simulating the T-Jump Triggered Unfolding Dynamics of Trpzip2 Peptide and its Time Resolved IR and 2DIR Signals Using Markov State Model Approach*", **J. Phys. Chem. B**. 115, 5415,(2011)
16) Bian, Hongtao; Li, Jiebo; Wen, Xiewen; Sun, Zhigang; Song, Jian; Wei Zhuang*; JR Zheng* "*Mapping Molecular Conformations with Multiple-Mode Two-Dimensional Infrared Spectroscopy*" **J. Phys. Chem. A.** 115, 3357,(2011)
17) W. Zhuang*, N. G. Sgourakis, A.E.Garcia and S. Mukamel *"Discriminating early stage Aβ42 monomer structures using chirality-induced 2DIR spectroscopy in a simulation study"* **Proceedings of National Academy of Sciences.USA,** 107 (36) 15687-15692(2010)
18) N. Sengupta, H. Maekawa, W. Zhuang, C. Toniolo, S. Mukamel, D.J. Tobias, and N.H. Ge *"Sensitivity of 2DIR spectra to peptide helicity: A concerted experimental and simulation study of an octopeptide"* **J. Phys. Chem. B,** 113, 12037 (2009)
19) W. Zhuang, T. Hayashi, S. Mukamel *"Coherent Multidimensional Vibrational Spectroscopy of Biomolecules; Concepts, Simulations and Challenges"* **Angew. Chem. Int. Edit.** 48, 3750 (2009)
20) S. Mukamel, W. Zhuang, D. Abramavicius and I. Schweigert *"Coherent spectroscopic probes of vibational and electronic correlations; from NMR to X rays"* **Accounts of Chemical Research,** 42, 553 (2009)
21) J. Wang, W. Zhuang, S. Mukamel and R. Hochstrasser *"Two-dimensional infrared spectroscopy as a probe of the solvent electrostatic field for a twelve residue peptide"* **J. Phys. Chem. B.** 112, 5930-5937 (2008)
22) V. Lorenz, W. Zhuang, S. Mukamel and Steve Cundiff *"Ultrafast Optical Spectroscopy of Spectral Fluctuations in a Dense Atomic Vapor"* **Phys. Rev. Lett.** 100, 013603 (2008)
23) Z. Li, H. Yu, W. Zhuang and S. Mukamel *"Geometry and Excitation Energy Fluctuations of NMA in Aqueous Solution with CHARMM, AMBER, OPLS, and GROMOS Force Fields: Implications for Protein Ultraviolet Spectra Simulation"* **Chem.Phys.Lett.** 452, 78 (2008)
24) C. Falvo, T. Hayashi, W. Zhuang, and S. Mukamel *"Coherent 2D spectroscopy of a cyclic decapeptide antamanide: A simulation study of the amide-I and amide-A bands"* **J. Phys. Chem. B,** 112, 12479 (2008)
25) V. Volkov, W. Zhuang, R. Chelli, F.Nuti, Y. Takaoka, A. Papini, S. Mukamel and R. Righini *"Electrostatic Interactions in Phospholipids Membranes Revealed by Coherent Two-Dimensional Infrared Spectroscopy"* **Proceedings of National Academy of Sciences.USA** (2007) 104 15323-15326
26) W.Zhuang, D. Abramavicius, D.Voronine and S. Mukamel *"Two-dimensional infrared spectroscopy of amyloid fibrils; structure determination complementary to solid state NMR"* **Proceedings of National Academy of Sciences.USA** (2007) 104 14233-14236
27) Z. Li, D. Abramavicius, W. Zhuang, and S. Mukamel *"Two Dimensional Electronic Correlation Spectroscopy of the npi* and pipi* Protein Backbone Transitions: A Simulation Study"* **Chemical Physics** (2007) 341, 29-36
28) W. Zhuang, D. Abramavicius, T. Hayashi and S. Mukamel *"Simulation Protocols for Coherent Femtosecond Vibrational Spectra of Peptides"* **J. Phys. Chem. B**, 2006, 110, 3362-3374.
29) D. Abramavicius, W. Zhuang, S. Mukamel *"Probing Molecular Chirality via Excitonic Nonlinear Response"* **J. Phys. B.** 39 (2006) 5051–5066.
30) W. Zhuang, D. Abramavicius, S. Mukamel *"Novel Two-Dimensional Vibrational Optical Probes for Peptide Fast Folding Investigation"* **Proceedings of National Academy of Sciences.USA** (2006) 103 18934–18938 **(highlighted by NATURE METHODS)**
31) T. Hayashi, T. Jansen, W. Zhuang, S. Mukamel, *"Collective Solvent Coordinates for the Infrared Spectrum of HOD in D2O Based on an Ab Initio Electrostatic Map,"* **J. Phys. Chem. B,** 2005, 109,

64-82.

32) W. Zhuang, D. Abramavicius and S. Mukamel *"Dissecting Coherent Vibrational Spectra of Small Proteins into Secondary Structural Elements by Sensitivity Analysis"* **Proceedings of National Academy of Sciences, USA.**2005, 102, 7443-7448
33) T. Jansen, T. Hayashi, W Zhuang and S. Mukamel *"Stochastic Liouville Equations for Hydrogen-Bonding Fluctuations and Their Signatures in Two-Dimensional Vibrational Spectroscopy of Water"* **J. Chem. Phys**. 2005, 123, 114504-114511.
34) S. Mukamel and W. Zhuang *"Coherent Femtosecond Multidimensional Probes of Molecular Vibrations"* **Proceedings of National Academy of Sciences, USA**. 2005, 102, 13717-13718.
35) T. Hayashi, W. Zhuang and S. Mukamel *"Electrostatic DFT Map for the Complete Vibrational Amide Band of NMA"* **J. Phys. Chem. A** 2005, 109, 9747-9759.
36) W. Zhuang and C. Dellago, "*Dissociation of Hydrogen Chloride and Proton Transfer in Liquid Glycerol: An Ab Initio Molecular Dynamics Study"*. **J. Phys. Chem. B. Special Issue "Frank H. Stillinger Festschrift"** 2004, 108, 19647-19656.
37) D. Abramavicius, W. Zhuang and S. Mukamel, *"Peptide Secondary Structure Determination by Three-Pulse Coherent Vibrational Spectroscopies; A Simulation Study,"* **J. Phys. Chem. B**, 2004, 108, 18034-18045.
38) T. Jansen, W. Zhuang, and S. Mukamel, *"Stochastic Liouville Equation Simulation of Multidimensional Vibrational Lineshapes of Trialanine,"* **J. Chem. Phys**. 2004,121, 10577-10598.

国内国际会议：

- "SPECTRON: A QM/MM Protocol for Simulating the Coherent 2D Vibrational Spectroscopy of Peptides" 美国化学学会年会 地点：美国佐治亚州亚特兰大 时间：2006年3月 （受邀）
- "Simulating the Chirality-Induced Coherent 2D Vibrational Spectroscopy of Peptides" 超快现象国际研讨会 地点：美国加州太平洋丛林市 时间：2006年7月
- "Multidimentional Spectroscopic probes for Biomolecules" 第五届国际华人理论与技术化学会议（WCTCC） 地点：厦门 时间：2009年9月.
- "2D Chiral Optical Spectroscopic Probes for Amyloid fibrils " 第二届手性振动光谱（VOA）和拉曼光谱的生物医学应用国际会议 地点：美国纽约奥尔巴尼 时间：2010年8月
- "Continuum Solvation Modeling in Biological Systems" 244届美国化学会年会地点：美国费城 时间：2012年8月
- "Functional Dynamics of Biomolecules - computational and experimental approaches"欧洲原子分子计算中心研讨会 地点：瑞士卢加诺 时间：2012年11月
- "Theoretical and Computational Chemistry"第六届亚太地区理论计算化学会议 地点：韩国庆州 时间：2013年7月