Wei Zhuang

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EDUCATION:

B.S in chemistry: University of Science and Technology of China 2000
M.S in chemistry: University of Rochester. 2003.
Ph.D. in chemistry: University of California, Irvine. 2007

RESEARCH INTERESTS:

- Developing a theoretical protocol for the modeling of nonlinear coherent optical signals combining molecular dynamics simulation, QM/MM Hamiltonian construction and Quasiparticle Green's function representation of the response.
- Bridging coherent optical spectroscopy with MD simulations.
- The application of ultrafast spectroscopies to peptide and protein folding, chemical exchange, light harvesting systems, membrane, biosensor and polymer materials.
- Coherent nonlinear spectroscopy theory and related fields: statistical mechanics, biophysics, quantum chemistry and many-body physics.

EXPERIENCE:

- 2001-2003: Working with Professor **Christoph Dellago** on statistical mechanics, classical and ab initio computer simulation.
- 2003-present: Working with Professor **Shaul Mukamel** on computer simulation and Modeling of ultrafast spectroscopy.
- 2003.10: Working with Professor **Ron Elber** on the Local Enhanced Sampling formalism and "MOIL" package.

SOFTWARE DEVELOPMENT AND APPLICATIONS:

- Main developer and coordinator of a C/C++ based (using FORTRAN90, LAPACK, FFTW3 and GSL) computational package **SPECTRON**: a user-friendly software for simulating optical spectra for biological systems and large scale materials, the code combines MD simulation with analytical models.
- Computer simulation formalisms and applications, Transition Path Sampling, Local Enhances Sampling, Umbrella Sampling, REMD, CPMD, CHARMM, AMBER, GROMOS,NAMD,TINKER.
- Quantum chemistry softwares: Gaussian, Gamess.
- Language Known: C/C++, Fortran, Tcl/Tk, Linux Bash, Tcsh. Perl and Python.

PRESENTATIONS:

- *"SPECTRON: A QM/MM Protocol for Simulating the Coherent 2D Vibrational Spectroscopy of Peptides"* **ACS Annual meeting,** Atlanta, GI, USA, March, 2006 (Invited talk)
- "*Simulating the Chirality-Induced Coherent 2D Vibrational Spectroscopy of Peptides*" **International Conference on Ultrafast Phenomena**, Pacific Grove, CA, USA, July, 2006.

PROPOSALS:

- Contributor of the NIH Proposal **"*Multidimensional Femtosecond Correlation Spectroscopic Probes of Biomolecules*"** (RO1-GM59230-05)

PUBLICATIONS:

1) 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.
2) 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.
3) 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.
4) T. Jansen, W. Zhuang, and S. Mukamel, *"Stochastic Liouville Equation Simulation of Multidimensional Vibrational Lineshapes of Trialanine,"* **J. Chem. Phys**. 2004,121, 10577-10598.
5) 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
6) 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.
7) S. Mukamel and W. Zhuang *"Coherent Femtosecond Multidimensional Probes of Molecular Vibrations"* **Proceedings of National Academy of Sciences, USA** 2005, 102, 13717-13718. (Editorial Material, mini review)
8) 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.
9) 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.
10) D. Abramavicius, W. Zhuang, S. Mukamel *"Probing Molecular Chirality via Excitonic Nonlinear Response"* **J. Phys. B. 39** (2006) 5051–5066.
11) 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
12) 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"* **(submitted to *NATURE*)**
13) W.Zhuang, D. Abramavicius, D.Voronine and S. Mukamel *"*Two-dimensional infrared spectroscopy of amyloid fibrils; structure determination complementary to solid state NMR*"* **(submitted to *NATURE*)**
14) W. Zhuang, J. Zheng, C. Dellago, M. Fayer and S. Mukamel *"Simulating Ultrafast Isomerization 2DIR spectrum using a combined protocol with CPMD, Transition Path Sampling and Stochastic Liouville Equation"* **(in preparation)**
15) J. Wang, W. Zhuang, R. Venkatramani, S. Mukamel and R. Hochstrasser *"Simulation of 2DIR spectrum of Isotope labeled Tryptophin Zipper 2 hairpin peptide based on a QM/MM modeling protocol"* **(in preparation)**

16) W. Zhuang, R. Venkatramani, J. Wang and S. Mukamel *"Simulation Protocols for Coherent Femtosecond Vibrational Spectra of Peptides II"* **(in preparation)**.
17) T. Hayashi, W. Zhuang, D. Abramavicius and S. Mukamel *"Vibrational-Exciton Couplings for Amide I, II, III and A Modes of Peptides"* **(in preparation)**
18) W. Zhuang and S. Mukamel *"Simulation Study of 2DIR signals for the Photochemically Triggered Azo-peptide Relaxation"* **(in preparation)**
19) W. Zhuang, and S. Mukamel *"Simulation Protocols for Peptide 2DIR spectroscopy"* (review paper) **(in preparation).**

Peer-Reviewed Conference Proceedings:

1) T. Hayashi, W. Zhuang and S. Mukamel *"Nonlinear Vibrational Responses of the Amide I, II, III and A Bands of NMA: Simulation Study Based on an Electrostatic DFT Map"* **International Conference on Time-Resolved Vibrational Spectroscopy (TRVS) XI ,** 2005**.**
2) W. Zhuang, D. Abramavicius and S. Mukamel *"Coherent Infrared Pulse Sequences for Probing Molecular Chirality"* **International Conference on Ultrafast Phenomena** . R.J.D. Miller, A.M. Weiner, P. Cornum and D.M. Jonas (editors) Springer Verlag (2006).
3) F. Sanda, W. Zhuang, T. Jansen, T. Hayashi and S. Mukamel *"Signatures of Chemical Exchange in 2D Vibrational Spectroscopy: Simulations Based on the Stochastic Liouville Equations"* **International Conference on Ultrafast Phenomena** . R.J.D. Miller, A.M. Weiner, P. Cornum and D.M. Jonas (editors) Springer Verlag (2006).
4) V. Lorenz, S. Cundiff, W. Zhuang and S. Mukamel."*Three-Pulse Photon Echo in a Dense Potassium Vapor*," **International Conference on Ultrafast Phenomena**, R.J.D. Miller, A.M. Weiner, P. Cornum and D.M. Jonas (editors) Springer Verlag (2006).
5) T. Hayashi, W. Zhuang and S. Mukamel."Lineshapes and Correlations in Two Dimensional Vibrational Signals of NMA", **International Conference on Ultrafast Phenomena**, R.J.D. Miller, A.M. Weiner, P. Cornum and D.M. Jonas (editors) Springer Verlag (2006).