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EDUCATION

2002	**Ph. D. Chemistry**	**The University of Tokyo** Prof. Hiro-o Hamaguchi Group	Tokyo, Japan
1999	**M. Sc. Chemistry**	**The University of Tokyo** Prof. Hiro-o Hamaguchi Group	Tokyo, Japan
1997	**B. Sc. Chemistry**	**The University of Tokyo** Prof. Mitsuo Tasumi Group	Tokyo, Japan

ACADEMIC POSITIONS

2008-Present:	Assistant Specialist,	**University of California, Davis**
	Advisor:	Prof. **Alexei Stuchebrukhov**
Sep.2008:	Invited Researcher,	**Kobe University**, Japan
	Host:	Prof. **Keisuke Tominaga**
2008:	Assistant Specialist,	**University of California, Irvine**
	Advisor:	Prof. **Shaul Mukamel**
Sep.2007:	Invited Researcher,	**Kobe University**, Japan
	Host:	Prof. **Keisuke Tominaga**
2003-2008:	Postdoctoral Researcher,	**University of California, Irvine**
	Advisor:	Prof. **Shaul Mukamel**
2002-2003:	Postdoctoral Researcher,	**University of Rochester**
	Advisor:	Prof. **Shaul Mukamel**

PROFESSIONAL SOCIETIES

- American Chemical Society
- Chemical Society of Japan
- Japan Society of Molecular Science
- Spectroscopical Society of Japan

RESEARCH SUMMARY

Assistant Specialist, *Prof. Alexei Stuchebrukhov Group*, UC, Davis (2008-present)

Long-distance Electron Tunneling in Proteins: Developed a code to calculate the electron tunneling pathways at atomic resolution, tunneling matrix elements, and electron transfer rates of long-distance electron tunneling in proteins. The code works in conjunction with Gaussian quantum chemistry package, and can thus be applicable at any computational level. The system studied is complex I, a key enzyme in the respiratory electron transport chain, which transfers electrons over 90 Å along seven Fe/S clusters. Complex I defects are the cause of many neurodegenerative diseases including Parkinson's disease. We for the first time identified distinct tunneling pathways, key protein residues, and proposed a unique role of internal water as a mediator.

Assistant Specialist, Prof, Shaul Mukamel Group, UC, Irvine (2003-2008)

Realistic Simulation of Anharmonic Vibrational Dynamics in Solution: Developed a new methodology for computationally efficient realistic simulation of the anharmonic vibrational dynamics of polyatomic molecules in solution (as an extension of my work in the graduate course). The model can treats vibrational dynamics such as dephasing, population transfer, exciton hopping, and correlated frequency fluctuations of multiple-quanta transitions of molecules as large as proteins based on a QM/MM scheme without repeating quantum mechanical (QM) calculations at each time step. The ab initio anhrmonic multi-dimensional vibrational Hamiltonian of QM regions (vibrational chromophores) is parameterized with respect to the local multipole electric field (denoted as Electronic DFT Maps). Coulombic interactions between QM regions are expanded in transition multipoles. By combining them with MD trajectories of the whole system and wave-propagation techniques, the vibrational dynamics of the whole system is obtained. The proposed technique is one of the most accurate and has been successfully applied to water (HOD/D_2O and pure H_2O) and many proteins, in good agreement with experiment. Simulations of the whole four amide vibrational regions (I, II, III and A) of proteins were performed for the first time.

2-Dimenstional Infrared Spectroscopy of Biomolecules: Applied the proposed technique to 2-Dimensinal infrared (2DIR) spectrsocopy. 2DIR has established itself as a useful tool for the investigation of the molecular structure and ultrafast molecular events due to its unique high temporal resolution and multidimensional spectral information although spectral analysis had been difficult because of the complexity of the Hamiltonian. We identified the 2DIR signatures of the extraordinary high anharmonicity of the malonaldehyde (a double-well type intramolecular proteon transfer system), correlations and excitonic couplings in the hydrogen-bond network of liquid water, correlated hydrogen bonding fluctuations at peptide amide bonds, and protein secondary structures. We demonstrated that 2DIR with polarized beams can distinguish multiple secondary structure candidates of a peptide which NMR cannot distinguish.

ACADEMIC CONTRIBUTIONS

- Referee for European Physical Journal

PUBLICATIONS IN PEER-REVIEWED JOURNALS **(>10 citations)**

1. **Tomoyuki Hayashi**, and Alexei Stuchebrukhov, "Electron Tunneling in Respiratory Complex I", ***Proc. Natl. Acad. Sci. USA*** (in press)
2. Shihai Yan, Sunwoo Kang, **Tomoyuki Hayashi**, Shaul Mukamel, and Jin Yong Lee, "Computational Studies on Electron and Proton Transfer in Phenol-Imidazole-Base Triads", ***J. Comp. Chem.*** 31, 393 (2010)
3. Wei Zhuang, **Tomoyuki Hayashi**, and Shaul Mukamel, "Coherent Multidimensional Vibrational Spectroscopy of Biomolecules; Concepts, Simulations and Challenges," ***Agnew Chem.*** 48, 3750 (2009) **(21 citations)**
4. Alex Paarmann, **Tomoyuki Hayashi**, Shaul Mukamel and R. J. Dwayne Miller, "Nonlinear response of vibrational excitons: Simulating the two-dimensional infrared spectrum of liquid water", ***J. Chem. Phys.*** 130, 204110 (2009)
5. **Tomoyuki Hayashi**, and Shaul Mukamel, "Two-Dimensional Vibrational Lineshapes of All Amide Bands in a Helical Peptide", ***J. Mol. Liq.*** 141, 149 (2008)
6. Alex Paarmann, **Tomoyuki Hayashi**, Shaul Mukamel and R. J. D. Miller, "Probing Intermolecular Couplings in Liquid Water with 2DIR Photon Echo Spectroscopy", ***J. Chem. Phys.*** 128, 191103 (2008) **(25 citations)**
7. Sayuri Yamaguchi, Motohiro Banno, Kaoru Ohta, Keisuke Tominagaa, and **Tomoyuki Hayashi**, "Vibrational dynamics of benzoic acid in nonpolar solvents studied by subpicosecond infrared pump–probe spectroscopy", ***Chem. Phys. Lett.*** 462, 238-242 (2008)
8. Cyril Falvo, **Tomoyuki Hayashi**, Wei Zhuang, and Shaul 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)
9. **Tomoyuki Hayashi**, and Shaul Mukamel, "Vibraion-exciton Couplings for the Amide I, II, III and A Modes of Peptides", ***J. Phys. Chem. B*** 111, 11032-11046 (2007) (**A Figure selected for Cover Art**) **(13 citations)**
10. Wei Zhuang, Darius. Abramavicius, **Tomoyuki Hayashi**, Shaul Mukamel, "Simulation Protocols for Coherent Femtosecond Vibrational Spectra of Peptides", ***J. Phys. Chem. B*** 110, 3362-3374 (2006) **(58 citations)**

11. **Tomoyuki Hayashi**, and Shaul Mukamel, "Correlated Hydrogen Bonding Fluctuations and Vibrational Cross Peaks in NMA: Simulation Based on a Complete Electrostatic DFT Map", ***J. Chem. Phys.*** 125, 194510-194520 (2006) (**Selected for December 1, 2006 issue of Virtual Journal of Biological Physics Research**) **(13 citations)**
12. **Tomoyuki Hayashi**, Thomas la Cour Jansen, Wei Zhuang, Shaul Mukamel, "Collective Solvent Coordinates for the Infrared Spectrum of HOD in D_2O Based on an Ab Initio Electrostatic Map", ***J. Phys. Chem. A,*** 109 64-82 (2005). **(69 citations)**
13. Thomas la Cour Jansen, **Tomoyuki Hayashi**, Wei Zhuang and Shaul Mukamel, "Stochastic Liouville Equations for Hydrogen-Bonding Fluctuations and their Signatures in Two Dimensional Vibrational Spectroscopy of Water", ***J. Chem. Phys.*** 123, 114504-114514 (2005) **(41 citations)**
14. **Tomoyuki Hayashi**, Wei Zhuang and Shaul Mukamel, "Electrostatic DFT Map for the Complete Vibrational Amide Band of NMA", ***J. Phys. Chem. A*** 109, 9747-9759 (2005) **(66 citations)**
15. **Tomoyuki Hayashi** and Shaul Mukamel, "Arnoldi Algorithm for the Simulation of Multidimensional Infrared Spectroscopy", ***Bull. Kor. Chem. Soc.*** 24, 1107-1110 (2003).
16. **Tomoyuki Hayashi** and Shaul Mukamel, "Multidimensional Infrared Signatures of Intramolecular Hydrogen-Bonding in Malonaldehyde", ***J. Phys. Chem. A*** 107, 9113-9131 (2003). **(34 citation)**
17. **Tomoyuki Hayashi**, and Shaul Mukamel, "Infrared Signatures of Proton Transfer in G.C and A.T Base Pairs: DFT Study", ***Israel J. Chem.*** 44, 185-191 (2003).
18. **Tomoyuki Hayashi**, and Hiro-o Hamaguchi, "Solvent Induced Dynamic Polarization, Vibrational Dephasing, and Infrared Band Shape of the C=O Stretch Mode of Acetone in Acetonitrile: a New Theoretical Approach", ***Chem. Phys. Lett.*** 326, 115-122 (1998) **(12 citations)**

UNREFEREED JOURNAL PUBLICATIONS AND CONFERENCE PAPERS

1. **Tomoyuki Hayashi,** "Simulational Approach to Vibrational Dyanmics in Solution and Its Application to 2-Dimensional Infrared Spectrosocpy" (in Japanese), *The Bulletin of the Molecular Simulation Society of Japan*, 11, 37-42 (2009)
2. **Tomoyuki Hayashi**, "Doing Research as a Post-doc in the USA" (in Japanese), *Molecular Science*, Vol. 1, No.1, A0014（2007）

3. Alex Paarmann, **Tomoyuki Hayashi**, Shaul Mukamel and R. J. Dwayne Miller,"Nonlinear Vibrational Response of Coupled Anharmonic System-Towards the 2DIR Spectrums of H2O," *TRVS Proceedings* (2007)
4. **Tomoyuki Hayashi**, Wei Zhuang, Shaul Mukamel, "Nonlinear Vibrational Response of the Amide I, II, III and A Bands of NMA: Simulation Study Based on an Electrostatic DFT Map", *TRVS XII Conference Proceeding*, (2006)
5. Frantisek Sanda, Wei Zhuang, Thomas La Cour Jansen, **Tomoyuki Hayashi** and Shaul Mukamel "Signatures of Chemical Exchange in 2D Vibrational Spectroscopy; Simulation Based on the Stochastic Liouville Equations", In *Ultrafast Phenomena XV*, R.J.D. Miller, A.M. Weiner, P. Cornum and D.M. Jonas (editors) Springer Verlag (2006)
6. **Tomoyuki Hayashi**, Wei Zhuang and Shaul Mukamel, "Lineshapes and Correlations in Two Dimensional Vibrational Signals of NMA", In *Ultrafast Phenomena XV*, R.J.D. Miller, A.M. Weiner, P. Cornum and D.M. Jonas (editors) Springer Verlag (2006)
7. **Tomoyuki Hayashi** and Shaul Mukamel, "Multidimensional Nonlinear Spectroscopy of Conformational Relaxation in Azobenzene", R. Venkatramani, *Ultrafast Phenomena XIII*, R.J.Miller, M.M. Murnane, N.F. Scherer, and A.M. Wiener, Editors (Springer-Verlag, Berlin) 619-621 (2002)

INVITED TALKS

1. **Tomoyuki Hayashi**, ”Simulational Study of Nonlinear Infrared Spectroscopy and Electron Tunneling of Proteins”, National Institute of Advanced Industrial Science and Technology (AIST), Japan, 2009/09
2. **Tomoyuki Hayashi**, “Introduction of Nonlinear Optical Spectroscopy” (3 consecutive 90min lectures for graduate students）, Kobe University, Japan, 2008/09/19-22
3. **Tomoyuki Hayashi**, ”Simulational Approach to Two Dimensional Infrared Spectroscopy”, 125th Physical Chemistry Seminar, Kobe University, Japan, 2008/09
4. **Tomoyuki Hayashi**, ”Introduction of Nonlinear Optical Spectroscopy”（3 consecutive 90min lectures for graduate students）, Kobe University, Japan, 2007/09/11-13
5. **Tomoyuki Hayashi**, ”Simulational Approach to Two Dimensional Infrared Spectroscopy”, Kobe University, Japan, 2007/09
6. **Tomoyuki Hayashi**, “Simulation of Two-dimensional Infrared Spectroscopy Based on Electrostatic DFT Map”, Institute for Molecular Science, Okazaki, 2006/08
7. **Tomoyuki Hayashi**, ”Simulated Studies of Two Dimensional Vibrational Spectroscopy Based on Electrostatic DFT Map”, 20th International Conference on Raman Spectroscopy, Yokohama, Japan, 2006/08
8. **Tomoyuki Hayashi**, “Boundary between the MD simulation, Spectroscopy and Liquid Chemistry”, 3rd Forum for Liquid Crystal Chemistry, Kanagawa Industrial Technology Research Institute, Japan, 2001/02

PRESENTATIONS IN THE U.S. AND INTERNATIONAL CONFERENCES

1. **Tomoyuki Hayashi**, Alexei Stuchebrukhov, "Electron Tunneling in Complex I of the Electron Transport Chain", Biomedical Computation at Stanford 2009 10th Annual Symposium, Stanford, U.S.A., 2009/11 [poster with a spotlight oral presentation]
2. **Tomoyuki Hayashi**, Protein dynamics and biological applications of time-resolved spectroscopy: A Satellite Meeting of the 20th International Conference on Raman Spectroscopy, Kobe, Japan, 2006/08 [poster]
3. **Tomoyuki Hayashi**, Zhuang Wei, Darius Abramavicious, Shaul Mukamel, "Lineshapes and Correlations in Two Dimensional Vibrational Signals of NMA", 20th International Conference on Ultrafast Phenomena, Pacific Grove, California, U.S.A., 2006/07 [poster]
4. **Tomoyuki Hayashi**, Wei Zhuang, Shaul Mukamel, "Electrostatic DFT Map for The Complete Vibrational Amide Band of NMA", American Conference on Theoretical Chemistry, Los Angeles, California, U.S.A., 2005/07 [poster]
5. **Tomoyuki Hayashi**, Hiro-o Hamaguchi,, 10th International Conference on Time-resolved Vibrational Spectroscopy, Okazaki, Japan, 2001/05 [poster]
6. **Tomoyuki Hayashi**, Hiro-o Hamaguchi, Gordon Research Conference on Vibrational Spectroscopy, Newport, Rhode Island, U.S.A., 2000/08 [poster]

PRESENTATIONS IN JAPAN

1. **Tomoyuki Hayashi**, and Alexei Stuchebrukhov, "Electron Tunneling in Respiratory Complex I", The 3rd Conference on Molecular Science, Osaka 2010/09[talk]
2. **Tomoyuki Hayashi**, "Simulation of Two-dimensional Infrared Spectroscopy of Glucose", The 2nd Conference on Molecular Science, Fukuoka, 2008/09[talk]
3. Sayuri Yamaguchi, Motohiro Banno, Kaoru Ohta, Keisuke Tominaga, **Tomoyuki Hayashi**, "Vibrational dynamics of benzoic acid in nonpolar solvents studied by subpicosecond infrared pump–probe spectroscop", 2nd Conveference on Molecular Science, Fukuoka, 2008/09 [talk]
4. **Tomoyuki Hayashi**, "Simulation of All Amide Vibrations of Peptides Based on Electrostatic DFT Map", The 1st Conference on Molecular Science, Sendai, 2007/09 [talk]
5. **Tomoyuki Hayashi**, Hiro-o Hamaguchi "Infrared Bandshape as a probe into Microscopic Fluctuations of Solvent in Solution – Solvent and Temperature Dependence of the Acetone C=O stretch vibrational bandshape", Conference on Molecular Structure in 2001, Sapporo, 2001/10 [talk]
6. **Tomoyuki Hayashi**, Hiro-o Hamaguchi, "Simulational Approach to Vibrational Dephasing and Infrared Bandshapes", IMS Symposium: Molecular Science of Peptides, Okazaki, 2000/12 [poster]
7. **Tomoyuki Hayashi**, Hiro-o Hamaguchi, "New Simulational Approach to Solvent Induced Dynamic Polarization, Vibrational Dephasing ", Conference on Molecular Structure, Tokyo, 2000/09 [poster]

8. **Tomoyuki Hayashi**, Hiro-o Hamaguchi, "Solvent Induced Dynamic Polarization, Vibrational Dephasing, and Infrared Band Shape of the C=O Stretch Mode of Acetone in Acetonitrile: a New Theoretical Approach", IMS Symposium: Current Situation and Future of Studies on Dynamics in Condensed Phase, Okazaki, 2000/06 [poster]
9. **Tomoyuki Hayashi**, Hiro-o Hamaguchi, 3rd Theoretical Chemistry Symposium, Kyoto, 1999/06 [poster]
10. **Tomoyuki Hayashi**, Hiro-o Hamaguchi, Conference on Molecular Structure in 1998, Matsuyama, 1998/10 [talk]

TEACHING EXPERIENCE

2008-Sep	Lecture for Graduate Students, ”Introduction to Nonlinear Optical Spectroscopy”, 3×90min, Kobe University , Japan
2007-Sep	Lecture for Graduate Students, ”Introduction to Nonlinear Optical Spectroscopy”, 3×90min, Kobe University , Japan

SKILLS AND EXPERIENCE IN COMPUTATIONAL CHEMISTRY

Programming Skills and Languages

- Object-oriented Programming for Large-scale Software Systems (Fortran 90, 95, 2003, C++, JAVA)
- Structured Programming (Fortran 77, C)
- MPI Parallel Computing
- Vector Optimization for Efficient Numerical Codes (Fortran, C, C++)
- Script Languages (Python, Perl, bash, csh, sh, etc)
- HTML

Programming Experiences

- A code to calculate the tunneling pathways, tunneling matrix elements, and electron transfer rates of long-distance electron tunneling in proteins, in conjunction with Gaussian package.
- Developed the core part of SPECTRON code which calculates linear and nonlinear infrared and electronic spectra of proteins based on a QM/MM method.
- Implementation of energy gradient at the Hartree-Fock, MPn and DFT level in presence of nonuniform multipole electric field to Gaussian 03 code.
- A molecular dynamics code for rigid body dynamics with Ewald summation and molecular polarization.
- A code to calculate anharmonic vibrational potential energy surface up to 6th order in multiple normal modes and to calculate eigenfunctions based on the vibrational configuration interaction (Vibrational CI). Arnoldi argorithm was used for the large scale matrix diagonalization.

- Developed a code to generate Electrostatic DFT Map (EDM): A map of spectroscopic properties (eigenfrequencies, transition dipole moments, equilibrium geometries) of a molecule with respect to multipole electric field generated by solvent.
- A code to calculate 2-dimensional infrared spectra from the proper combination of 4-point dipole correlation functions with the cumulant expansion of Gaussian fluctuations.

Calculation Experiences

- Quantum Chemical Calculations: Gaussian and GAMESS
- Molecular dynamics Simulations: GROMACS, CHARMM and NAMD

Familiar Operating Systems and Administrations:

- Linux, UNIX, Windows, and Mac OS
- Administrator of Linux PC clusters and web servers in Shaul Mukamel and Alexei Stuchebrukhov groups.

PERSONAL INFORMATION

Nationality:	Japanese Citizen
Gender:	Male
Date of Birth:	August 31st, 1973
Place of Birth:	Tokyo
Marital Status:	Married with two children

LANGUAGES

English:	Fluent in speaking and writing.
Japanese:	Native

REFERENCES

Alexei A. Stuchebrukhov, Ph. D. stuchebr@chem.ucdavis.edu
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University of California, Davis
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Mitsuo Tasumi, Ph. D. tasumi@sapiarc.com
Professor Emeritus, Dept. Chemistry, The University of Tokyo
Former Visiting Professor, College of Chemistry, University of California Berkeley
Former President, Saitama University