

## ANDREI TOKMAKOFF – CURRICULUM VITAE

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### Education

1988 B.S. in Chemistry, California State University, Sacramento  
1991 M.S. in Chemistry, Stanford University  
1995 Ph.D. in Chemistry, Stanford University. Research Advisor: Michael D. Fayer

### Positions and Employment

1995-96 Alexander von Humboldt Research Fellow, Technical University, Munich  
1996-98 NSF Postdoctoral Fellow, Univ. of Chicago and James Franck Institute, and UC Berkeley and Lawrence Berkeley National Lab  
1998-03 Assistant Professor, Department of Chemistry, Massachusetts Institute of Technology  
2003-07 Associate Professor, Department of Chemistry, Massachusetts Institute of Technology  
2007-12 Professor of Chemistry, Department of Chemistry, Massachusetts Institute of Technology  
2012 Robert T. Haslam and Bradley Dewey Professor of Chemistry, Mass. Institute of Technology  
2013- Henry G. Gale Distinguished Service Professor, Department of Chemistry, James Franck Institute, and Institute for Biophysical Dynamics, University of Chicago

### Honors and Awards

1994 Alexander von Humboldt Foundation Research Fellowship  
1995 National Science Foundation Postdoctoral Fellowship in Chemistry  
1999 Research Corporation Research Innovation Award  
2000 David and Lucile Packard Fellowship for Science and Engineering  
2001 Richard E. Heikkila Research Scholar Award (National Parkinson Foundation)  
2001 Outstanding Young Investigator (Time-Resolved Vibrational Spectroscopy Conference)  
2002 National Fresenius Award (Phi Lambda Upsilon)  
2002 Alfred P. Sloan Research Fellowship  
2002 Coblentz Award (Coblentz Society)  
2009 Fellow of the Optical Society of America  
2012 Ernest K. Plyler Prize for Molecular Spectroscopy (American Physical Society)  
2014 Ellis R. Lippincott Award (Optical Society of America)  
2016 Ahmed Zewail Award in Ultrafast Science and Technology (American Chemical Society)

### Professional Activities and Societies

Faculty advisor to 26 graduate students, 12 postdoctoral scholars, and 17 undergraduate students  
Patents: 4 granted (US 7,696,479; 7,812,311; 8,526,002; 9,476,768), 2 provisional filings  
Core MIT Faculty: Harrison Spectroscopy Lab (1999-2012), Laser Biomedical Research Facility (2010-2012)  
MIT Biophysics Program Committee (2009-2012)  
UChicago Biophysics Graduate Program Committee (2013-2015)  
Member: Amer. Chem. Society, Biophysical Society, Optical Society of America (OSA), Protein Society

Ad Hoc Reviewer: DOE Site Review Panel, Argonne (1999), RIKEN Molecular Spectroscopy Lab (2015), NIH Special Emphasis Panel/SRG (2008, 2010)

Visiting Member: NIH MSFB Study Section (2011 and 2016)

Symposium Organizer/Co-Organizer: OSA Frontiers in Optics/Laser Science Meeting, October 2004; APS Nat'l Meeting, March 2005; ACS Nat'l Meeting, March 2008; APS Nat'l Meeting, March 2015.

Conference Committees: Int'l. Conf. on Ultrafast Phenomena, 2004-2008; Int'l. Conf. on Coherent Multidimensional Spectroscopy, 2004-pres.; Int'l. Conf. on Time-Resolved Vibrational Spectroscopy, 2005-pres.

Conference Chair: 14th International Conference on Time-Resolved Vibrational Spectroscopy, 2009.

Editorial Committees: *Advances in Chemical Physics* (2007-2016); *Annual Reviews of Physical Chemistry* (2007-2012); *Journal of Chemical Physics* (2008-2010); *Chemical Science* (2012-2013); *Journal of Physical Chemistry* (2013-2015).

Guest Editor/Co-Editor: *Journal of Chemical Physics*, Special Issue on Biological Water (2014).

Advisory Committee: Munich-Centre for Advanced Photonics (2008-2011).

Scientific Advisory Board: Max-Born-Institute, Berlin, Germany (2011-2015).

## Publications since 2012

1. "Transient two-dimensional spectroscopy with linear absorption corrections applied to temperature-jump two-dimensional infrared," K. C. Jones, Z. Ganim, C. Sam Peng, and A. Tokmakoff, *J Opt Soc Am B*, **29** (2012) 118–129.
2. "Coherent two-dimensional infrared spectroscopy: Quantitative analysis of protein secondary structure in solution," Carlos Baiz, Chunte Sam Peng, Michael E. Reppert, Kevin C. Jones, and Andrei Tokmakoff, *Analyst*, **137** (2012) 1793-1799.
3. "Identifying residual structure in intrinsically disordered systems: A 2D IR spectroscopic study of the GVGXPGVG peptide," Joshua Lessing, Santanu Roy, Mike Reppert, Marcel Baer, Dominik Marx, Thomas La Cour Jansen, J. Knoester, and A. Tokmakoff, *J Am Chem Soc*, **134** (2012) 5032–5035.
4. "A phenomenological approach to modeling chemical dynamics in nonlinear and two-dimensional spectroscopy," Krupa Ramasesha, Luigi De Marco, Andrew D. Horning, Aritra Mandal and Andrei Tokmakoff, *J Chem Phys*, **136** (2012) 134507-1-11.
5. "An Introduction to Protein 2D IR Spectroscopy," Carlos Baiz, Mike Reppert, Andrei Tokmakoff, in *Ultrafast Infrared Vibrational Spectroscopy*, ed. by M. D. Fayer (Taylor & Francis, New York, 2013).
6. "Heterogeneous folding of a  $\beta$ -hairpin peptide revealed through temperature-jump 2D IR spectroscopy," Kevin C. Jones, Chunte Sam Peng and Andrei Tokmakoff, *PNAS USA*, **110** (2013) 2828-2833.
7. "Identification of lactam-lactim tautomers of aromatic heterocycles in aqueous solution using 2D IR spectroscopy," Chunte Sam Peng and Andrei Tokmakoff, *J Phys Chem Letters*, **3** (2012) 3302-3306.
8. "Amide I Two-Dimensional Infrared Spectroscopy: Methods for Visualizing the Vibrational Structure of Large Proteins," Carlos Baiz, Mike Reppert, Andrei Tokmakoff, *J Phys Chem A*, **117** (2013) 5955-5961.
9. "Cooperative Cold Denaturation: The Case of the C-terminal Domain of the Ribosomal Protein L9," Bowu Luan, Bing Shan, Carlos Baiz, Andrei Tokmakoff, and Daniel P. Raleigh, *Biochemistry*, **52** (2013) 2402-2409.
10. "Electrostatic Frequency Shifts in Amide I Vibrational Spectra: Direct Parameterization against Experiment," Mike Reppert and Andrei Tokmakoff, *J Chem Phys*, **138** (2013) 134116-1-11.
11. "Direct Observation of Ground State Lactam–Lactim Tautomerization Using Temperature-Jump Transient 2D IR Spectroscopy," Chunte Sam Peng, Carlos R. Baiz, and Andrei Tokmakoff, *PNAS USA*, **110** (2013) 9243-9248.

12. "Direct Observation of Multiple Tautomers of Oxythiamine and their Recognition by the Thiamine Pyrophosphate Riboswitch," Vipender Singh, Chunte Sam Peng, Deyu Li, Koyel Mitra, Katherine J Silvestre, Andrei Tokmakoff, and John Essigmann, *ACS Chem Biol*, **9** (2014) 227-236.
13. "Water vibrations have strongly mixed intra- and inter-molecular character," Krupa Ramasesha, Luigi De Marco, Aritra Mandal, and Andrei Tokmakoff, *Nature Chem*, **5** (2013) 935-940.
14. "Experimental evidence for Fermi resonances in isotopically dilute water from ultrafast broadband IR spectroscopy," Luigi De Marco, Krupa Ramasesha, and Andrei Tokmakoff, *J Phys Chem B*, **117** (2013) 15319-15327.
15. "A Molecular Interpretation of 2D IR Protein Folding Experiments with Markov State Models," Carlos R. Baiz, Yu-Shan Lin, Chunte Sam Peng, Kyle A. Beauchamp, Vincent A. Voelz, Vijay S. Pande, and Andrei Tokmakoff, *Biophys J*, **106** (2014) 1359-1370.
16. "Robust Excitations Inhabit Supra-molecular Light-Harvesting Nanotubes," Dörthe M. Eisele, Dylan H. Arias, Xiaofeng Fu, Erik A. Bloemsma, Colby P. Steiner, Russell A. Jensen, Patrick Rebentrost, Holger Eisele, Andrei Tokmakoff, Seth Lloyd, Keith A. Nelson, Daniela Nicastro, Jasper Knoester, and Mounqi G. Bawendi, *PNAS USA*, **111** (2014) E3367-E3375.
17. "Tautomerism provides a molecular explanation for the mutagenic properties of the anti-HIV nucleoside analog 5-aza-5,6-dihydro-2'-deoxycytidine," Deyu Li, Bogdan I. Fedeles, Vipender Singh, Chunte Sam Peng, Katherine J. Silvestre, Allison K. Simi, Jeffrey H. Simpson, Andrei Tokmakoff and John M. Essigmann, *PNAS USA*, **111** (2014) E3252-E3259.
18. "Collective Vibrations of Water-Solvated Hydroxide Ions Investigated with Broadband 2DIR Spectroscopy," Aritra Mandal, Krupa Ramasesha, Luigi De Marco and Andrei Tokmakoff, *J Chem Phys*, **140** (2014) 204508-1-12.
19. "Local and Collective Reaction Coordinates in the Transport of the Aqueous Hydroxide Ion," Sean T. Roberts, Aritra Mandal and Andrei Tokmakoff, *J Phys Chem B*, **118** (2014) 8062-8069.
20. "Two-dimensional IR spectroscopy of the anti-HIV agent KP1212 reveals protonated and neutral tautomers that influence pH-dependent mutagenicity," C. S. Peng, B. I. Fedeles, V. Singh, D. Li, T. Amariuta, J. M. Essigmann, and A. Tokmakoff, *PNAS USA*, **112** (2015) 3229-3234.
21. "Direct Observation of Intermolecular Interactions Mediated by Hydrogen Bonding," Luigi De Marco, Martin Thämer, Mike Reppert, and Andrei Tokmakoff, *J Chem Phys*, **141** (2014) 034502-1-10.
22. "Ultrafast 2D IR microscopy," Carlos R. Baiz, Denise Schach, and Andrei Tokmakoff, *Opt Express*, **22** (2014) 18724-18735.
23. "Structural characterization of folded protein ensembles: Isotope-edited 2D IR spectroscopy and spectral simulations based on a Markov state model," Carlos Baiz and Andrei Tokmakoff, *Biophys J*, **108** (2015) 1747-1757.
24. "Preface: Special Topic on Biological Water," Gerhard Hummer and Andrei Tokmakoff, *J Chem Phys*, **141** (2014) 22D101-1-2.
25. "Visualizing KcsA Conformational Changes upon Ion Binding by Infrared Spectroscopy and Atomistic Modeling," Paul Stevenson, Christoph Götz, Carlos R. Baiz, Jasper Akerboom, Andrei Tokmakoff, and Alipasha Vaziri, *J Phys Chem B* **119** (2015) 5824-5831.
26. "Isotope-Enriched Protein Standards for Computational Amide I Spectroscopy," Mike Reppert, Anish R. Roy, and Andrei Tokmakoff, *J Chem Phys*, **142** (2015) 125104-1-10.
27. "Distinguishing Gramicidin D Conformers through Two-Dimensional Infrared Spectroscopy of Vibrational Excitons," Paul Stevenson and Andrei Tokmakoff, *J Chem Phys*, **142** (2015) 212424.
28. "Communication: Quantitative multi-site frequency maps for amide I vibrational spectroscopy," Mike Reppert and Andrei Tokmakoff, *J Chem Phys*, **143** (2015) 061102.
29. "Ultrafast 2D IR spectroscopy of the excess proton in liquid water," Martin Thämer, Luigi De Marco, Krupa Ramasesha, Aritra Mandal, Andrei Tokmakoff, *Science*, **350** (2015) 78-82.

30. "Vibrational Dynamics of Aqueous Hydroxide Solutions Probed using Broadband 2DIR Spectroscopy," Aritra Mandal and Andrei Tokmakoff, *J Chem Phys*, **143** (2015) 194501-1-10.
31. "Weakened N3 Hydrogen Bonding by 5-Formylcytosine and 5-Carboxylcytosine Reduces Their Base-Pairing Stability," Qing Dai, Paul J. Sanstead, Chunte Sam Peng, Dali Han, Chuan He, Andrei Tokmakoff, *ACS Chem Biol*, **11** (2016) 477-477.
32. "Computational Amide I 2D IR Spectroscopy as a Probe of Protein Structure and Dynamics," Mike Reppert and Andrei Tokmakoff, *Annu Rev Phys Chem*, **67** (2016) 359-386.
33. "Role of Pre-Solvation and Anharmonicity in Aqueous Phase Hydrated Proton Solvation and Transport," Rajib Biswas, Ying-Lung Steve Tse, Andrei Tokmakoff, and Gregory A. Voth, *J Phys Chem B*, **120** (2016) 1793-1804.
34. "Efficient Total Chemical Synthesis of  $^{13}\text{C}=^{18}\text{O}$  Isotopomers of Human Insulin for Isotope-Edited FTIR," Balamurugan Dhayalan, Ann Fitzpatrick, Kalyaneswar Mandal, Jonathan Whittaker, Michael A. Weiss, Andrei Tokmakoff, and Stephen B. H. Kent, *ChemBioChem*, **17** (2016) 415-420.
35. "Crystallization of Enantiomerically Pure Proteins from Quasi-Racemic Mixtures: Structure Determination by X-Ray Diffraction of Isotope-Labeled Ester Insulin and Human Insulin," Kalyaneswar Mandal, Balamurugan Dhayalan, Michal Avital-Shmilovici, Andrei Tokmakoff, and Stephen B. H. Kent, *ChemBioChem*, **17** (2016) 421-425.
36. "Differences in the Vibrational Dynamics of  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$ : Observation of Symmetric and Antisymmetric Stretching Vibrations in Heavy Water," Luigi De Marco, William Carpenter, Hanchao Liu, Rajib Biswas, Joel M. Bowman, and Andrei Tokmakoff, *J Phys Chem Lett*, **7** (2016) 1769-1774.
37. "Studying Protein-Protein Binding through T-Jump Induced Dissociation: Transient 2D IR Spectroscopy of Insulin Dimer," Xin-Xing Zhang, Kevin C. Jones, Ann Fitzpatrick, Chunte Sam Peng, Chi-Jui Feng, Carlos Baiz, and Andrei Tokmakoff, *J Phys Chem B*, **120** (2016) 5134-5145.
38. "Interplay of Ion-Water and Water-Water Interactions within the Hydration Shells of Nitrate and Carbonate Directly Probed with 2D IR Spectroscopy," Joseph A. Fournier, William Carpenter, Luigi De Marco, and Andrei Tokmakoff, *J Am Chem Soc*, **138** (2016) 9634-9645.
39. "Sequence-Dependent Mechanism of DNA Oligonucleotide Dehybridization Resolved through Infrared Spectroscopy," Paul J. Sanstead, Paul Stevenson, and Andrei Tokmakoff, *J Am Chem Soc*, **138** (2016) 11792-11801.
40. "Anharmonic exciton dynamics and energy dissipation in liquid water from two-dimensional infrared spectroscopy," Luigi De Marco, Joseph A. Fournier, Martin Thämer, William Carpenter, and Andrei Tokmakoff, *J Chem Phys*, **145** (2016) 094501-1-13.
41. "Refining Disordered Peptide Ensembles with Computational Amide I Spectroscopy: Application to Elastin-Like Peptides," Mike Reppert, Anish R. Roy, Jeremy O. B. Tempkin, Aaron R. Dinner, and Andrei Tokmakoff, *J Phys Chem B*, **120** (2016) 11395-11404.
42. "Molecular Modeling and Assignment of IR Spectra of the Hydrated Excess Proton in Isotopically Dilute Water," Rajib Biswas, William Carpenter, Gregory Voth, and Andrei Tokmakoff, *J Chem Phys*, **145** (2016)