

## 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  
2018-21 Chair, Department of Chemistry, 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)  
2017 Distinguished Service Award, California State University Sacramento  
2018 American Academy of Arts and Sciences  
2022 National Academy of Sciences

### Professional Activities and Societies

Faculty advisor to 38 graduate students, 17 postdoctoral scholars, and 19 undergraduate students  
Patents: 5 granted (US 7,696,479; 7,812,311; 8,526,002; 9,222,881; 9,476,768), 1 filing  
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: American Chemical Society, Biophysical Society, Optica, Protein Society  
Ad Hoc Reviewer: DOE Site Review Panel, Argonne (1999), NIH Special Emphasis Panel/SRG (2008, 2010), RIKEN Molecular Spectroscopy Lab (2015), NSF CHE Panel (2018, 2022)  
Review Panel Chair: IBS Center for Molecular Spectroscopy and Dynamics, Seoul, South Korea (2020)  
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: Annual Reviews of Physical Chemistry (2007-2012); Advances in Chemical Physics (2007-2016); Journal of Chemical Physics (2008-2010); Chemical Science (2012-2019); Journal of Physical Chemistry (2013-2015, 2022-2025).  
Guest Editor/Co-Editor: Journal of Chemical Physics, Special Issue on Biological Water (2014).  
Advisory Committee: Munich-Centre for Advanced Photonics (2008-2014)  
Scientific Advisory Board: Max-Born-Institute, Berlin, Germany (2011-2015).

## Publications since 2018

1. "Fourier Transform Fluorescence-Encoded Infrared Spectroscopy," Joseph N. Mastron and Andrei Tokmakoff, *J Phys Chem A*, **122** (2018) 554-562.
2. "Picosecond Proton Transfer Kinetics in Water Revealed with Ultrafast IR Spectroscopy," William B. Carpenter, Joseph A. Fournier, Nicholas H.C. Lewis, and Andrei Tokmakoff, *J Phys Chem B*, **122** (2018) 2792-2802.
3. "Infrared Insights into the Effect of Cholesterol on Lipid Membranes," Paul Stevenson and Andrei Tokmakoff, *Chem Phys*, **512** (2018) 146-153.
4. "Broadband 2D IR spectroscopy reveals dominant asymmetric  $\text{H}_5\text{O}_2^+$  proton hydration structures in acid solutions," Joseph A. Fournier, William B. Carpenter, Nicholas H.C. Lewis, and Andrei Tokmakoff, *Nat Chem*, **10** (2018) 932-937.
5. "Direct Observation of Activated Kinetics and Downhill Dynamics in DNA Dehybridization," Paul J. Sanstead and Andrei Tokmakoff, *J Phys Chem B*, **122** (2018) 3088-3100.
6. "Single stage MHz mid-IR OPA using  $\text{LiGaS}_2$  and a fiber laser pump source," Samuel Penwell, Lukas Whaley-Mayda, and Andrei Tokmakoff, *Opt Lett*, **43** (2018) 1363-1366.
7. "Refinement of Peptide Conformational Ensembles by 2D IR Spectroscopy: Application to Ala-Ala-Ala," Chi-Jui Feng, Balamurugan Dhayalan, and Andrei Tokmakoff, *Biophys J*, **114** (2018) 2820-2832.
8. "Direct Observation of Ion Pairing in Aqueous Nitric Acid Using 2D Infrared Spectroscopy," Nicholas H.C. Lewis, Joseph A. Fournier, William B. Carpenter, and Andrei Tokmakoff, *J Phys Chem B*, **123** (2019), 225-238.
9. "Length-Dependent Melting Kinetics of Short DNA Oligonucleotides Using Temperature-Jump IR Spectroscopy," Ryan J. Menssen and Andrei Tokmakoff, *J Phys Chem B*, **123** (2019) 756-767.
10. "A Lattice Model for the Interpretation of Oligonucleotide Hybridization Experiments," Paul J. Sanstead and Andrei Tokmakoff, *J Chem Phys*, **150** (2019) 185104-1-12.
11. "Fluorescence Encoded Infrared Spectroscopy: Ultrafast Vibrational Spectroscopy on Small Ensembles of Molecules in Solution," Lukas Whaley-Mayda, Samuel Penwell, and Andrei Tokmakoff, *J Phys Chem Lett*, **10** (2019) 1967-1972.

12. "Entropic Barriers in the Kinetics of Aqueous Proton Transfer," William B. Carpenter, Nicholas H.C. Lewis, Joseph A. Fournier, and Andrei Tokmakoff, *J Chem Phys*, **151** (2019) 034501-1-11.
13. "High-Level VSCF/VCI Calculations Decode the Vibrational Spectrum of the Aqueous Proton," Qi Yu, William B. Carpenter, Nicholas H. C. Lewis, Andrei Tokmakoff, Joel M. Bowman, *J Phys Chem B*, **123** (2019) 7214-7224.
14. "5-Carboxylcytosine and Cytosine Protonation Uniquely Influence Dehybridization of the DNA Duplex," Brennan Ashwood, Paul Sanstead, Qing Dai, Chuan He, Andrei Tokmakoff, *J Phys Chem B*, **124** (2020) 627-640.
15. "Signatures of Ion-Pairing and Aggregation in the Vibrational Spectroscopy of Super-Concentrated Aqueous Lithium Bistriflimide Solutions," Nicholas H. C. Lewis, Yong Zhang, Bogdan Dereka, Emily V. Carino, Edward J. Maginn, and Andrei Tokmakoff, *J Phys Chem C*, **124** (2020) 3470-3481.
16. "Oxidized Derivatives of 5-Methylcytosine Alter the Stability and Dehybridization Dynamics of Duplex DNA," Paul Sanstead, Brennan Ashwood, Qing Dai, Chuan He, Andrei Tokmakoff, *J Phys Chem B*, **124** (2020) 1160-1174.
17. "Dynamic and programmable cellular-scale granules enable tissue-like materials," Yin Fang, Endao Han, Xin-Xing Zhang, Yuanwen Jiang, Yiliang Lin, Jiuyun Shi, Jiangbo Wu, Lingyuan Meng, Xiang Gao, Philip J. Griffin, Xianghui Xiao, Hsiu-Ming Tsai, Hua Zhou, Xiaobing Zuo, Qing Zhang, Miaoqi Chu, Qingteng Zhang, Ya Gao, Leah K. Roth, Reiner Bleher, Zhiyuan Ma, Zhang Jiang, Jiping Yue, Chien-Min Kao, Chin-Tu Chen, Andrei Tokmakoff, Jin Wang, Heinrich M. Jaeger, Bozhi Tian, *Matter*, **2** (2020) 948-964.
18. "Revealing the Dynamical Role of Co-solvents in the Coupled Folding and Dimerization of Insulin," Xin-Xing Zhang and Andrei Tokmakoff, *J Phys Chem Lett* **11** (2020) 4353-4358.
19. "Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction," Carlos R. Baiz, Bartosz Błasiak, Jens Bredenbeck, Minhaeng Cho, Jun-Ho Choi, Steven A. Corcelli, Arend G. Dijkstra, Chi-Jui Feng, Sean Garrett-Roe, Nien-Hui Ge, Magnus W. D. Hanson-Heine, Jonathan D. Hirst, Thomas L. C. Jansen, Kijeong Kwac, Kevin J. Kubarych, Casey H. Londergan, Hiroaki Maekawa, Mike Reppert, Shinji Saito, Santanu Roy, James L. Skinner, Gerhard Stock, John E. Straub, Megan C. Thielges, Keisuke Tominaga, Andrei Tokmakoff, Hajime Torii, Lu Wang, Lauren J. Webb, and Martin T. Zanni, *Chem Rev*, **120** (2020) 7152-7218.
20. "Vibrational Probe of Aqueous Electrolytes: The Field Is Not Enough," Nicholas H. C. Lewis, Aysenur Iscen, Alanna Felts, Bogdan Dereka, George C. Schatz, and Andrei Tokmakoff, *J Phys Chem B*, **124** (2020) 7013-7026.
21. "Temperature-Jump 2D IR Spectroscopy with Intensity-Modulated CW Optical Heating," Brennan Ashwood, Nicholas H.C. Lewis, Paul J. Sanstead, and Andrei Tokmakoff, *J Phys Chem B*, **124** (2020) 8665-8677.
22. "Insulin Dissociates by Diverse Mechanisms of Coupled Unfolding and Unbinding," Adam Antoszewski, Chi-Jui Feng, Bodhi P. Vani, Erik H. Thiede, Lu Hong, Jonathan Weare, Andrei Tokmakoff, and Aaron R. Dinner, *J Phys Chem B*, **27** (2020) 5571-5587.
23. "DNA minor-groove binder Hoechst 33258 destabilizes base-pairing adjacent to its binding site," Xin-Xing Zhang, Shelby Brantley, Steven Corcelli, and Andrei Tokmakoff, *Commun Biol*, **3** (2020) 525.
24. "Decoding the 2D IR spectrum of the aqueous proton with high-level VSCF/VCI calculations," William B. Carpenter, Qi Yu, John H. Hack, Bogdan Dereka, Joel M. Bowman, and Andrei Tokmakoff, *J Chem Phys*, **153** (2020) 124506.
25. "Temperature-Jump 2D IR Spectroscopy with Intensity-Modulated CW Optical Heating," Brennan Ashwood, Nicholas H. C. Lewis, Paul J. Sanstead, Andrei Tokmakoff, *Journal of Physical Chemistry B*, **124** (2020) 8665-8677.

26. "Crossover from Hydrogen to Chemical Bonding," Bogdan Dereka, Qi Yu, Nicholas H. C. Lewis, William B. Carpenter, Joel M. Bowman, Andrei Tokmakoff, *Science*, **371** (2021) 160-164. DOI: 10.1126/science.abe1951
27. "Investigation into the Mechanism and Dynamics of DNA Association and Dissociation Utilizing Kinetic Monte Carlo Simulations," Ryan Menssen, Gregory Kimmel, and Andrei Tokmakoff, *Journal of Chemical Physics*, **154**, (2021) 045101-1-13.
28. "Fluorescence-Encoded Infrared Vibrational Spectroscopy with Single-Molecule Sensitivity," Lukas Whaley-Mayda, Abhirup Guha, Samuel Penwell, and Andrei Tokmakoff, *Journal of the American Chemical Society*, **143** (2021) 3060–3064.
29. "Computational IR Spectroscopy of Insulin Dimer Structure and Conformational Heterogeneity," Chi-Jui Feng, Anton Sinitskiy, Vijay Pande, and Andrei Tokmakoff, *Journal of Physical Chemistry B*, **125** (2021) 4620–4633.
30. "Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport," Edward Barry, et al. *Chemical Reviews*, **121** (2021) 9450–9501.
31. "Water-in-Salt LiTFSI Aqueous Electrolytes (I): Liquid Structure from Combined Molecular Dynamics Simulation and Experimental Studies," Yong Zhang, Nicholas Lewis, Julian Mars, Gang Wan, Nickolas Weadock, Christopher Takacs, Maria Lukatskaya, Hans-Georg Steinrück, Michael Toney, Andrei Tokmakoff, Edward Maginn, *Journal of Physical Chemistry B*, **125** (2021) 4501–4513.
32. "Structural characterization of protonated water clusters confined in HZSM-5 zeolites," John H. Hack<sup>†</sup>, James P. Dombrowski<sup>†</sup>, Xinyou Ma<sup>†</sup>, Yaxin Chen, Nicholas H. C. Lewis, William B. Carpenter, Chenghan Li, Gregory A. Voth, Harold H. Kung and Andrei Tokmakoff, *Journal of the American Chemical Society*, **143** (2021) 10203–10213.
33. "Determining sequence-dependent DNA oligonucleotide hybridization and dehybridization mechanisms using coarse-grained molecular simulation, Markov state models, and infrared spectroscopy," Michael S. Jones, Brennan Ashwood, Andrei Tokmakoff, and Andrew L. Ferguson, *Journal of the American Chemical Society*, **143** (2021) 17395-17411.
34. "Water or Anion? Uncovering Zn<sup>2+</sup> Solvation Environment in Mixed Zn(TFSI)<sub>2</sub> and LiTFSI Water-in-Salt Electrolytes," Yong Zhang<sup>†</sup>, Gang Wan<sup>†</sup>, Nicholas H. C. Lewis<sup>†</sup>, Julian Mars, Sharon E. Bone, Hans-Georg Steinrück, Maria R. Lukatskaya, Nicholas J. Weadock, Michal Bajdich, Oleg Borodin, Andrei Tokmakoff, Michael F. Toney, and Edward J. Maginn, *ACS Energy Letters*, **6** (2021) 3458–3463.
35. "Structural ensemble of the insulin monomer," Luis Busto-Moner, Chi-Jui Feng, Adam Antoszewski, Andrei Tokmakoff, and Aaron R. Dinner, *Biochemistry*, **60** (2021) 3125–3136.
36. "Lineshape Distortions in Internal Reflection 2DIR Spectroscopy: Tuning Across the Critical Angle," Nicholas H. C. Lewis and Andrei Tokmakoff, *Journal of Physical Chemistry Letters*, **12** (2021) 11843–11849.
37. "Characterization of Acetonitrile Isotopologues as Vibrational Probes of Electrolytes," Bogdan Dereka, Nicholas H. C. Lewis, Jonathan H. Keim, Scott A. Snyder, Andrei Tokmakoff, *The Journal of Physical Chemistry B*, **126** (2022) 278–291.
38. "Exchange-Mediated Transport in Battery Electrolytes: Ultrafast or Ultraslow?" Bogdan Dereka, Nicholas H. C. Lewis, Yong Zhang, Nathan Hahn, Jonathan H. Keim, Scott A. Snyder, Edward Maginn, Andrei Tokmakoff, *Journal of the American Chemical Society*, **144** (2022) 8591–8604.
39. "Resonance conditions, detection quality, and single-molecule sensitivity in fluorescence-encoded infrared vibrational spectroscopy," Lukas Whaley-Mayda, Abhirup Guha, and Andrei Tokmakoff, *Journal of Chemical Physics*, **156** (2022) 174202.
40. "From Networked to Isolated: Observing Water Hydrogen Bonds in Concentrated Electrolytes with Two-Dimensional Infrared Spectroscopy," Nicholas H. C. Lewis, Bogdan Dereka, Yong Zhang, Edward J. Maginn, and Andrei Tokmakoff, *Journal of Physical Chemistry B* **126** (2022) 5305–5319.