

MIKE REPPERT

Department of Chemistry \diamond University of Toronto
80 St. George Street \diamond Toronto, ON, Canada
647-636-4919 \diamond mreppert@alum.mit.edu

EDUCATION

Massachusetts Institute of Technology <i>PhD in Physical Chemistry under Andrei Tokmakoff</i>	Cambridge, MA 04/2016
Kansas State University <i>BS in Chemistry, Biochemistry, and Mathematics</i>	Manhattan, KS 05/2009

RESEARCH EXPERIENCE

University of Toronto <i>Postdoctoral Fellow</i>	Toronto, ON, Canada 01/2017 -
--	----------------------------------

Open quantum systems theory with Paul Brumer focusing on quantum effects in light-activated biological processes. Areas of expertise: Quantum/classical master equations, semiclassical quantization, molecular dynamics.

University of Stuttgart <i>Postdoctoral Researcher</i>	Stuttgart, Germany 10/2016 - 12/2016
--	---

Nonequilibrium statistical mechanics under Matthias Krüger, focusing on driven particle dynamics under nonlinear friction. Areas of expertise: Langevin dynamics, Stochastic differential equations, nonlinear response theory.

University of Chicago <i>Graduate Research Assistant</i>	Chicago, IL 05/2013 - 05/2016
--	----------------------------------

Thesis research under Andrei Tokmakoff developing quantitative methods for protein vibrational spectroscopy simulations and structural ensemble refinement. Areas of expertise: IR spectroscopy, recombinant expression, peptide synthesis, molecular dynamics, maximum entropy methods.

Massachusetts Institute of Technology <i>Graduate Research Assistant</i>	Cambridge, MA 09/2010 - 04/2013
--	------------------------------------

Thesis research under Andrei Tokmakoff focusing on the simulation of linear and nonlinear infrared spectroscopy. Areas of expertise: 2D IR spectroscopy, molecular dynamics, C/Python/Matlab programming.

Institute of Physics, Polish Academy of Sciences <i>Fulbright Scholar</i>	Warsaw, Poland 10/2009 - 05/2010
---	-------------------------------------

Single-molecule spectroscopy and lineshape theory under Bolesław Kozankiewicz. Areas of expertise: Single-molecule spectroscopy, fluorescence line narrowing.

Kansas State University <i>Undergraduate Research Assistant</i>	Manhattan, KS 08/2005 - 05/2009
---	------------------------------------

Low-temperature optical spectroscopy of photosynthetic proteins under Ryszard Jankowiak. Areas of expertise: Hole burning spectroscopy, photosynthetic antenna proteins, Scilab programming.

Ames Laboratory, US DOE <i>Undergraduate Research Assistant</i>	Ames, IA 06/2005 - 07/2005
---	-------------------------------

Low-temperature spectroscopy with Ryszard Jankowiak. Areas of expertise: ring-dye lasers.

AWARDS AND HONORS

- Banting Postdoctoral Fellowship 2017 -
- U. Toronto Faculty of Arts and Science Postdoctoral Fellowship Award 2017 -
- Weatherford Energy Fellowship 2010 - 2011
- NSF Graduate Research Fellowship 2009 - 2014
- Fulbright U.S. Student Grant 2009 - 2010
- KSU Presidential Award for Distinguished Undergraduate Student in Research 2008
- Goldwater Scholarship 2007 - 2009
- National Merit Scholarship 2004 - 2008

TEACHING EXPERIENCE

Biophysical Chemistry (5.64) Massachusetts Institute of Technology
Grader Spring 2012

Generated solutions, graded assignments, and delivered a guest lecture on the biophysics of photosynthesis.

Thermodynamics and Kinetics (5.60) Massachusetts Institute of Technology
Graduate Teaching Assistant Fall 2010 - Spring 2011

Held bi-weekly recitation sections and graded homework and exams for 10 - 20 students. Net student evaluation ratings were 6.2 and 6.1 (scale of 1 to 7) for Fall 2010 and Spring 2011.

Real Number Systems (Math 521) Kansas State University
Grader Fall 2008

Generated solutions and graded homework papers in introductory number theory.

PROFESSIONAL ACTIVITIES AND SERVICES

Undergraduate/High School Research Mentor U. Chicago / KSU
Mentor 2007 - 2016

Mentored one high-school/undergraduate student under Ryszard Jankowiak (KSU) and three undergraduate researchers under Andrei Tokmakoff (U. Chicago). Supervised activities include project design, programming, lab work, and publication of results.

Physics with a Bang University of Chicago
Presenter 12/2014

Built and presented for local elementary school students a demonstration on stroboscopic measurements using a strobe light, dark hood, and falling water droplets coupled to a bass speaker.

Summer Mini-course in Nonlinear Spectroscopy University of Chicago
Lecturer 07/2013

Presented an informal one-month lecture series on nonlinear spectroscopy attended by departmental graduate students, undergraduates, and postdoctoral researchers.

Chemistry High School Symposium Kansas State University
Organizing Committee Member 05/2007 and 04/2008

Planned and organized activities, seminars, and lab tours for high school students; oversaw student registration and communication; presented and led discussion on undergraduate research.

SELECTED ORAL PRESENTATIONS

- “Quantum or Classical? The Case of 2D Vibrational Spectroscopy,” Quantum Frontiers in Molecular Science Workshop, Telluride, CO, June 27, 2018.
- “Classical Beats: A Classical Framework for Multidimensional Spectroscopy,” 100th Canadian Chemistry Conference and Exhibition, Toronto, ON, Canada, May 29, 2017.
- “Proteins out of Order: Building and Benchmarking New Tools to Study Disordered Peptide Ensembles,” Purdue University Physical Chemistry Seminar Series, West Lafayette, IN, March 30, 2016.
- “Computational Amide I Spectroscopy for Refinement of Disordered Peptide Ensembles: Maximum Entropy and Related Approaches,” American Physical Society March Meeting, Baltimore, MD, March 15, 2016.
- “Hole Burning in Excitonically Coupled Systems: Modeling and Interpretation of Experimental Data,” University of Tartu, Tartu, Estonia, June 17, 2011.
- “Modeling of Hole Burning Spectra in Photosynthetic Systems,” University of Leiden, Leiden, Netherlands, May 6, 2010.
- “Monte Carlo Simulations of Non-Resonant Hole Burning Spectra: Applications to Photosynthetic Complexes,” Technical University of Berlin, Berlin, Germany, September 28, 2009. Related work presented at Adam Mickiewicz University (Poznan, Poland, Oct. 2), the PAN Center of Molecular and Macromolecular Studies (Łódź, Poland, Nov. 5), and the PAN Institute of Physics (Warsaw, Poland, Nov. 24).
- “Simulation of Hole-Burned Spectra of the CP43 Proximal Antenna Complex of Higher Plant Photosystem II,” 42nd Midwest Regional Meeting of the ACS, Kansas City, MO, November 8, 2007.

PUBLICATIONS

- [1] **Reppert, M.** and Brumer, P. Quantumness in light harvesting is determined by vibrational dynamics. *J. Chem. Phys.* **149**(23), 234102 (2018).
- [2] **Reppert, M.** and Brumer, P. Classical Coherent Two-dimensional Vibrational Spectroscopy. *J. Chem. Phys.* **148**(6), 064101 (2018).
- [3] **Reppert, M.**, Roy, A. R., Tempkin, J. O. B., Dinner, A. R., and Tokmakoff, A. Refining Disordered Peptide Ensembles with Computational Amide I Spectroscopy: Application to Elastin-Like Peptides. *J. Phys. Chem. B* **120**(44), 11395–11404 (2016).
- [4] **Reppert, M.** and Tokmakoff, A. Computational Amide I 2D IR Spectroscopy as a Probe of Protein Structure and Dynamics. *Ann. Rev. Phys. Chem.* **67**(1), 359–386 (2016).
- [5] **Reppert, M.** and Tokmakoff, A. Communication: Quantitative multi-site frequency maps for amide I vibrational spectroscopy. *J. Chem. Phys.* **143**(6), 061102 (2015).
- [6] **Reppert, M.**, Roy, A. R., and Tokmakoff, A. Isotope-enriched protein standards for computational amide I spectroscopy. *J. Chem. Phys.* **142**(12), 125104 (2015).
- [7] **Reppert, M.**, Kell, A., Pruitt, T., and Jankowiak, R. Comments on the optical lineshape function: Application to transient hole-burned spectra of bacterial reaction centers. *J. Chem. Phys.* **142**(9), 094111 (2015).

- [8] Vrandečić, K., Rätsep, M., Wilk, L., Rusevich, L., Golub, M., **Reppert, M.**, Irrgang, K.-D., Kühlbrandt, W., and Pieper, J. Protein Dynamics Tunes Excited State Positions in Light-Harvesting Complex II. *J. Phys. Chem. B* **119**(10), 3920–3930 (2015).
- [9] De Marco, L., Thämer, M., **Reppert, M.**, and Tokmakoff, A. Direct observation of intermolecular interactions mediated by hydrogen bonding. *J. Chem. Phys.* **141**(3), 034502 (2014).
- [10] Lin, C., **Reppert, M.**, Feng, X., and Jankowiak, R. Modeling of fluorescence line-narrowed spectra in weakly coupled dimers in the presence of excitation energy transfer. *J. Chem. Phys.* **141**(3), 035101 (2014).
- [11] Baiz, C., **Reppert, M.**, and Tokmakoff, A. An Introduction to Protein 2D IR Spectroscopy. In *Ultrafast Infrared Vibrational Spectroscopy*, Fayer, M., editor, chapter 12, 361–404. Taylor & Francis, Boca Raton (2013).
- [12] Kell, A., Feng, X., **Reppert, M.**, and Jankowiak, R. On the Shape of the Phonon Spectral Density in Photosynthetic Complexes. *J. Phys. Chem. B* **117**(24), 7317–7323 (2013).
- [13] Baiz, C. R., **Reppert, M.**, and Tokmakoff, A. Amide I Two-Dimensional Infrared Spectroscopy: Methods for Visualizing the Vibrational Structure of Large Proteins. *J. Phys. Chem. A* **117**(29), 5955–5961 (2013).
- [14] **Reppert, M.** and Tokmakoff, A. Electrostatic frequency shifts in amide I vibrational spectra: Direct parameterization against experiment. *J. Chem. Phys.* **138**(13), 134116 (2013).
- [15] Acharya, K., Zazubovich, V., **Reppert, M.**, and Jankowiak, R. Primary Electron Donor(s) in Isolated Reaction Center of Photosystem II from *Chlamydomonas reinhardtii*. *J. Phys. Chem. B* **116**(16), 4860–4870 (2012).
- [16] Baiz, C. R., Peng, C. S., **Reppert, M. E.**, Jones, K. C., and Tokmakoff, A. Coherent two-dimensional infrared spectroscopy: Quantitative analysis of protein secondary structure in solution. *Analyst* **137**, 1793–1799 (2012).
- [17] Lessing, J., Roy, S., **Reppert, M.**, Baer, M., Marx, D., Jansen, T. L. C., Knoester, J., and Tokmakoff, A. Identifying Residual Structure in Intrinsically Disordered Systems: A 2D IR Spectroscopic Study of the GVGXPGVG Peptide. *J. Am. Chem. Soc.* **134**(11), 5032–5035 (2012).
- [18] Neupane, B., Jaschke, P., Saer, R., Beatty, J. T., **Reppert, M.**, and Jankowiak, R. Electron Transfer in *Rhodobacter sphaeroides* Reaction Centers Containing Zn-Bacteriochlorophylls: A Hole-Burning Study. *J. Phys. Chem. B* **116**(10), 3457–3466 (2012).
- [19] **Reppert, M.** Modeling of Resonant Hole-Burning Spectra in Excitonically Coupled Systems: The Effects of Energy-Transfer Broadening. *J. Phys. Chem. Lett.* **2**(21), 2716–2721 (2011).
- [20] Jankowiak, R., **Reppert, M.**, Zazubovich, V., Pieper, J., and Reinot, T. Site Selective and Single Complex Laser-Based Spectroscopies: A Window on Excited State Electronic Structure, Excitation Energy Transfer, and Electron-Phonon Coupling of Selected Photosynthetic Complexes. *Chem. Rev.* **111**(8), 4546–4598 (2011).
- [21] **Reppert, M.**, Acharya, K., Neupane, B., and Jankowiak, R. Lowest Electronic States of the CP47 Antenna Protein Complex of Photosystem II: Simulation of Optical Spectra and Revised Structural Assignments. *J. Phys. Chem. B* **114**(36), 11884–11898 (2010).
- [22] **Reppert, M.**, Naibo, V., and Jankowiak, R. Accurate modeling of fluorescence line narrowing difference spectra: Direct measurement of the single-site fluorescence spectrum. *J. Chem. Phys.* **133**(1), 014506 (2010).

- [23] Acharya, K., Neupane, B., **Reppert, M.**, Feng, X., and Jankowiak, R. On the Unusual Temperature-Dependent Emission of the CP47 Antenna Protein Complex of Photosystem II. *J. Phys. Chem. Lett.* **1**(15), 2310–2315 (2010).
- [24] Neupane, B., Dang, N. C., Acharya, K., **Reppert, M.**, Zazubovich, V., Picorel, R., Seibert, M., and Jankowiak, R. Insight into the Electronic Structure of the CP47 Antenna Protein Complex of Photosystem II: Hole Burning and Fluorescence Study. *J. Am. Chem. Soc.* **132**(12), 4214–4229 (2010).
- [25] **Reppert, M.**, Naibo, V., and Jankowiak, R. Modeling study of non-line-narrowed hole-burned spectra in weakly coupled dimers and multi-chromophoric molecular assemblies. *Chem. Phys.* **367**, 27–35 (2010).
- [26] **Reppert, M.**, Naibo, V., and Jankowiak, R. Analytical formulas for low-fluence non-line-narrowed hole-burned spectra in an excitonically coupled dimer. *J. Chem. Phys.* **131**(23), 234104 (2009).
- [27] **Reppert, M.**, Zazubovich, V., Dang, N. C., Seibert, M., and Jankowiak, R. Low-Energy Chlorophyll States in the CP43 Antenna Protein Complex: Simulation of Various Optical Spectra. II. *J. Phys. Chem. B* **112**(32), 9934–9947 (2008).
- [28] Dang, N. C., Zazubovich, V., **Reppert, M.**, Neupane, B., Picorel, R., Seibert, M., and Jankowiak, R. The CP43 Proximal Antenna Complex of Higher Plant Photosystem II Revisited: Modeling and Hole Burning Study. I. *J. Phys. Chem. B* **112**(32), 9921–9933 (2008).
- [29] Dang, N. C., Reinot, T., **Reppert, M.**, and Jankowiak, R. Temperature Dependence of Hole Growth Kinetics in Aluminum-Phthalocyanine-Tetrasulfonate in Hyperquenched Glassy Water. *J. Phys. Chem. B* **111**(7), 1582–1589 (2007).
- [30] Miksa, B., Chinnappan, R., Dang, N. C., **Reppert, M.**, Matter, B., Tretyakova, N., Grubor, N. M., and Jankowiak, R. Spectral Differentiation and Immunoaffinity Capillary Electrophoresis Separation of Enantiomeric Benzo(a)pyrene Diol Epoxide-Derived DNA Adducts. *Chem. Res. Toxicol.* **20**(8), 1192–1199 (2007).

REFERENCES

Prof. Paul Brumer

University of Toronto
 Department of Chemistry
 80 St. George Street
 LM 421B
 Toronto, ON M5S 3H6
 Canada
 416-978-3569
 pbrumer@chem.utoronto.ca

Prof. Andrei Tokmakoff

University of Chicago
 Department of Chemistry
 929 E. 57th Street
 GCIS E139D
 Chicago, IL 60637
 773-834-7696
 tokmakoff@uchicago.edu

Prof. Ryszard Jankowiak

Kansas State University
 Department of Chemistry
 213 CBC Building
 Manhattan, KS 66506-0401
 785-532-6785
 ryszard@k-state.edu