Joel D. Eaves, Ph.D.

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Education

Postdoctoral Scientist
Columbia University, 2005-2008.
Postdoctoral advisor: David R. Reichman

Ph.D. Chemistry
Massachusetts Institute of Technology, 2005.
Advisor: Andrei Tokmakoff
Thesis title: "Vibrational Dynamics in Water from the Molecule's Perspective."

B.S. Physics
University of Wisconsin, Madison, 1999.

B.S. Chemistry
University of Wisconsin, Madison, 1999.

Research Interests

Condensed phase theoretical chemistry. Ultrafast vibrational and electronic dynamics in molecules and nanostructures including singlet fission and vibrational dephasing; aqueous transport across two-dimensional crystals; carrier dynamics in semiconducting nanostructures; magnetic and opto-electronic properties of iron sulfur solids and nanostructures; spontaneous self-organization in active matter systems; glassy dynamics; force-structure-function relationships at the mesoscale in DNA.

Honors and Awards

Student-selected "Best Physical Chemistry Seminar of the Spring Semester," University of Wisconsin, Madison (2016)

NSF CAREER Award (2015).

Walter A. Rosenblith Graduate Fellowship, MIT (1999).

Emil Fischer Award, U.W. Madison (1998).

Hilldale Research Award, U.W. Madison (1998).

Present Appointment

Associate Professor — 8/17–present
Department of Chemistry and Biochemistry, — Boulder, Colorado
University of Colorado, Boulder

Previous Appointments and Research Experience

Assistant Professor — 8/09–7/17
Department of Chemistry and Biochemistry, — Boulder, Colorado
University of Colorado, Boulder

Co-founder 1/09–7/09
Director of Research and Development
ThinkEco, Inc. New York, NY
Co-founder of a cleantech startup focused on domestic electrical energy conservation. Managed a small team of scientists and engineers through several versions of hardware and software prototypes, granted one US patent, negotiated pilot tests at Harvard and MIT, helped secure venture funding.

Postdoctoral Scientist 2005–2008
David R. Reichman Columbia University
Theories of reaction–subdiffusion for intracellular enzyme kinetics, ultrafast coherent energy transfer, and the dynamics of supercooled liquids in four spatial dimensions.

Graduate Research Assistant 1999–2005
Andrei Tokmakoff Massachusetts Institute of Technology
Ultrafast spectroscopy of liquids and molecular dynamics simulations to study equilibrium hydrogen bond dynamics in liquid water.

Undergraduate Research Assistant 1996–1999
F. Fleming Crim University of Wisconsin
Designed and built an optically coupled acoustic device to measure high resolution spectra of corrosive gases.

Research Assistant 1995
Gaea Technologies Princeton, New Jersey
Speckle interferometry to detect microscopic structural defects in load-bearing structures.

Publications

Research Articles

1. Strong, S. E. & Eaves, J. D. Linear Response Theory for Water Transport Through Dry Nanopores. *The Journal of Physical Chemistry A* **121**(29), 5377–5382. 10.1021/acs.jpca.7b03192 (2017).
2. Strong, S. E. & Eaves, J. D. The Dynamics of Water in Porous Two-Dimensional Crystals. *The Journal of Physical Chemistry B* **121**(1), 189–207. 10.1021/acs.jpcb.6b09387 (2017).
3. Utterback, J. K., Grennell, A. N., Wilker, M. B., Pearce, O. M., Eaves, J. D. & Dukovic, G. Observation of Trapped-hole Diffusion on the Surfaces of CdS Nanorods. *Nature Chemistry* **8,** 1061–1066. 10.1038/nchem.2566 (2016).
4. Strong, S. E. & Eaves, J. D. Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Graphene. *Journal of Physical Chemistry Letters* **7**(10), 1907–1912. 10.1021/acs.jpclett.6b00748 (2016).
5. Atkin, J. M., Sass, P. M., Teichen, P. E., Eaves, J. D. & Raschke, M. B. Nanoscale Probing of Dynamics in Local Molecular Environments. *Journal of Physical Chemistry Letters* **6**(22), 4616–4621. 10.1021/acs.jpclett.5b02093 (2015).
6. Teichen, P. E. & Eaves, J. D. Collective Aspects of Singlet Fission in Molecular Crystals. *The Journal of Chemical Physics* **143**(4), 044118. http://dx.doi.org/10.1063/1.4922644 (2015).
7. Price, A. C., Pilkiewicz, K. R., Graham, T. G. W., Song, D., Eaves, J. D. & Loparo, J. J. DNA Motion Capture Reveals the Mechanical Properties of DNA at the Mesoscale. *Biophysical Journal* **108**(10), 2532–2540. 10.1016/j.bpj.2015.04.022 (2015).
8. Strong, S. E. & Eaves, J. D. Tetracene Aggregation on Polar and Nonpolar Surfaces: Implications for Singlet Fission. *Journal of Physical Chemistry Letters* **6**(7), 1209–1215. 10.1021/acs.jpclett.5b00141 (2015).

9. Utterback, J. K., Wilker, M. B., Brown, K. A., King, P. W., Eaves, J. D. & Dukovic, G. Competition between Electron Transfer, Trapping, and Recombination in CdS Nanorod-hydrogenase Complexes. *Physical Chemistry Chemical Physics* **17**(8), 5538–5542. 10.1039/C4CP05993J (2015).
10. Pilkiewicz, K. R. & Eaves, J. D. Reentrance in an Active Glass Mixture. *Soft Matter* **10**(38), 7495–7501. 10.1039/C4SM01177E (2014).
11. Sweeney, M. C. & Eaves, J. D. Exciton Dynamics in Carbon Nanotubes: From the Luttinger Liquid to Harmonic Oscillators. *Physical Review Letters* **112**(10), 107402. 10.1103/PhysRevLett.112.107402 (2014).
12. Pilkiewicz, K. R. & Eaves, J. D. Flocking with Minimal Cooperativity: The Panic Model. *Physical Review E* **89**(1), 012718. 10.1103/PhysRevE.89.012718 (2014).
13. Ostrowski, J. H. J. & Eaves, J. D. The Tunable Hydrophobic Effect on Electrically Doped Graphene. *Journal of Physical Chemistry B* **118**(2), 530–536. 10.1021/jp409342n (2014).
14. Teichen, P. E. & Eaves, J. D. A Microscopic Model of Singlet Fission. *Journal of Physical Chemistry B* **116**(37), 11473–11481. 10.1021/jp208905k (2012).
15. Sweeney, M. C. & Eaves, J. D. Carrier Transport in Heterojunction Nanocrystals Under Strain. *Journal of Physical Chemistry Letters* **3**(6), 791–795. 10.1021/jz201368e (2011).
16. Eaves, J. D. & Reichman, D. R. Spatial Dimension and the Dynamics of Supercooled Liquids. *Proceedings of the National Academy of Sciences* **106**(36), 15171–15175. 10.1073/pnas.0902888106 (2009).
17. Jang, S., Cheng, Y.-C., Reichman, D. R. & Eaves, J. D. Theory of Coherent Resonance Energy Transfer. *Journal of Chemical Physics* **129**(10), 101104. 10.1063/1.2977974 (2008).
18. Eaves, J. D. & Reichman, D. R. The Subdiffusive Targeting Problem. *Journal of Physical Chemistry B* **112**(14), 4283–4289. 10.1021/jp0749017 (2008).
19. Eaves, J. D., Tokmakoff, A. & Geissler, P. L. Electric Field Fluctuations Drive Vibrational Dephasing in Water. *Journal of Physical Chemistry A* **109**(42), 9424–9436. 10.1021/jp051364m (2005).
20. Eaves[1], J. D., Loparo[1], J. J., Fecko, C. J., Roberts, S. T., Tokmakoff, A. & Geissler, P. L. Hydrogen Bonds in Liquid Water are Broken only Fleetingly. *Proceedings of the National Academy of Sciences of the United States of America* **102**(37), 13019–13022. 10.1073/pnas.0505125102 (2005).
21. Harder[1], E., Eaves[1], J. D., Tokmakoff, A. & Berne, B. J. Polarizable Molecules in the Vibrational Spectroscopy of Water. *Proceedings of the National Academy of Sciences of the United States of America* **102**(33). 10.1073/pnas.0505206102 (2005).
22. Loparo, J. J., Fecko, C. J., Eaves, J. D., Roberts, S. T. & Tokmakoff, A. Reorientational and Configurational Fluctuations in Water Observed on Molecular Length Scales. *Physical Review B* **70**(18), 180201. 10.1103/PhysRevB.70.180201 (2004).
23. Fecko[1], C. J., Eaves[1], J. D., Loparo, J. J., Tokmakoff, A. & Geissler, P. L. Ultrafast Hydrogen-Bond Dynamics in the Infrared Spectroscopy of Water. *Science* **301**(5640), 1698–1702. 10.1126/science.1087251 (2003).
24. Eaves, J. D., Fecko, C. J., Stevens, A. L., Peng, P. & Tokmakoff, A. Polarization-selective Femtosecond Raman Spectroscopy of Low-frequency Motions in Hydrated Protein Films. *Chemical Physics Letters* **376**(1), 20–25. 10.1016/S0009-2614(03)00890-X (2003).
25. Fecko, C. J., Eaves, J. D. & Tokmakoff, A. Isotropic and Anisotropic Raman Scattering from Molecular Liquids Measured by Spatially Masked Optical Kerr Effect Spectroscopy. *Journal of Chemical Physics* **117**(3), 1139–1154. 10.1063/1.1485070 (2002).

Patents

1. Shimada, J., Shibata, M., and Eaves, J. D., System and Method for Monitoring and Management of Utility Usage. US 8,433,530 B2, Published Mar. 18, 2010.

[1]First author paper with equal author contributions; typically joint experimental/theoretical effort.

Peer-reviewed conference proceedings

1. Teichen, P. E. & Eaves, J. D. Quantum Relaxation in Singlet Fission. *Bulletin of the American Physical Society* **58**(1), N38.00006 (2013).
2. Sweeney, M. C. & Eaves, J. D. Vortices in One Dimension: A Soliton Analysis of Gapped Carbon Nanotubes. *APS March Meeting Abstracts* **58**(1), N5.00008 (2013).
3. Teichen, P. E. & Eaves, J. D. Adiabatic and Nonadiabatic Dynamics in Singlet Fission. *Abstracts of Papers of the American Chemical Society* **243** (2012).
4. Loparo, J. J., Fecko, C. J., Eaves, J. D., Roberts, S. T., Geissler, P. L. & Tokmakoff, A. Probing Ultrafast Hydrogen Bond Dynamics on Water's Energy Landscape. *Abstracts of Papers of the American Chemical Society* **229,** U718 105–PHYS Part 2 (2005).
5. Fecko, C. J., Loparo, J. J., Eaves, J. D., Geissler, P. L. & Tokmakoff, A. Hydrogen Bond Dynamics in Water: Vibrational Echoes and 2D IR Spectroscopy. *Abstracts of Papers of the American Chemical Society* **227,** U256–U256 68–PHY Part 2 (2004).

Invited Presentations

1. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Physical Chemistry/Chemcial Physics Seminar. University of Colorado. Boulder, CO. September 8, 2017.
2. "Collective Aspects of Singlet Fission," Quantum Effects in the Condensed Phase, TSRC. Telluride, CO. July 25, 2017.
3. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Chemistry Coloquium. Columbia University. New York, NY. April 27, 2017.
4. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Physical Chemistry Seminar. University of Kansas. Lawrence, Kansas. March 31, 2017.
5. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Physical Chemistry Seminar. University of Southern California. Los Angeles, California. March 18, 2017.
6. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Physical Chemistry Seminar. University of California, Irvine. Irvine, California. March 17, 2017.
7. "Chemistry as a Matter of Scale," Physical Chemistry Seminar. California Institute of Technology. Pasadena, California. Nov 27, 2016.
8. "Chemistry as a Matter of Scale," Physical Chemistry Seminar. University of California, Berkeley. Berkeley, California. October 11, 2016.
9. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Physical Chemistry Seminar. Northwestern University. Evanston, Illinois. September 26, 2016.
10. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," James Franck Institute Seminar. University of Chicago. Chicago, Illinois. May 31, 2016.
11. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Physical Chemistry Seminar. Stanford University. Palo Alto, California. April 12, 2016.
12. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Harvard/MIT/BU Greater Boston Area Theoretical Chemistry Seminar. Massachusetts Institute of Technology (MIT). Cambridge, Massachusetts. April 27, 2016.
13. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Physical Chemistry Seminar. University of Wisconsin, Madison. Madison, Wisconsin. March 1, 2016.

14. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Physical Chemistry Seminar. Colorado State University. Fort Collins, Colorado. November 3, 2016.
15. "Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two-Dimensional Crystals," Physical Chemistry Seminar. University of Texas, Austin. Austin, Texas. February 18, 2016.
16. "Quantum and Classical Liquids," Telluride Science Research Center (TSRC), *New Challenges for Theory in Chemical Dynamics*. Telluride, Colorado. January 10–15, 2016.
17. "Molecular and Collective Motions in Singlet Fission," Physical Chemistry Seminar. University of California, San Diego (UCSD). San Diego, California. April 7, 2015.
18. "Water on Graphene: Tuning Hydrophobicity and Transport," Gordon Research Conference, *Physics and Chemistry of Liquids*. Holderness, New Hampshire. August 2–7, 2015.
19. "Singlet Fission in the Condensed Phase: Special Features of Molecular Crystals," American Chemical Society (ACS), *Computational Spectroscopy*. San Fransisco, California. August 13, 2014.
20. "The Hydrophobic Effect at Electrically Doped Graphene and Applications to Reverse Osmosis," Telluride Science Research Center (TSRC), *Hydrophobicity: From Theory and Simulation to Experiment*. Telluride, Colorado. June 24–28, 2014.
21. "Quantum and Classical Liquids," Physical Chemistry Seminar. University of Washington, Seattle. Seattle, Washington. March 3, 2014.
22. "Carrier Dynamics in the Face of Strong Interactions," Telluride Science Research Center (TSRC), *Advances in Photoreactions: When Spin-orbit Coupling, Optical Excitation, and Motion of Nuclei are of Equal Importance?* Telluride, Colorado. June 28, 2013.
23. "Carrier Transport in Nanoscale Heterojunctions Under Strain," Molecular Reaction Dynamics Symposium, in Honor of F. F. Crim. University of Wisconsin, Madison. Madison, Wisconsin. May 25, 2012.
24. "Carrier Dynamics in the Face of Strong Interactions," Theoretical Chemistry Institute Seminar. University of Wisconsin, Madison. Madison, Wisconsin. May 7, 2012.
25. "Transport in Heterojunction Nanocrystals Under Strain," Physical Chemistry Seminar. Colorado State University. Fort Collins, Colorado. November 3, 2011.
26. "Life in the Trenches: Glassy Dynamics in Liquids and Biology," Condensed Matter Physics Seminar. University of Colorado, Boulder. Boulder, Colorado. September 10, 2009.

Contributed Presentations

1. "The Virtue of Being Crystalline: Kinetics and Quantum Decoherence in Singlet Fission," 3rd Singlet Fission Workshop. Lyons, Colorado. June 16–18, 2013.
2. "Singlet Fission," 2nd Second Singlet Fission Workshop. Lyons, Colorado. June 17–20, 2012.
3. "A Microscopic Model for Singlet Fission," 1st Singlet Fission Workshop. Golden, Colorado. May 9–10, 2011.

Teaching Experience

1. Chemistry 4531 *Physical Chemistry II*, University of Colorado, 1 semester. Fall 2017: Modernized subject matter to include computation, differential equations, and waves.
2. Chemistry 4555/5555 *Theoretical and Computational Chemistry*, University of Colorado, 2 semesters. Fall 2015, Spring 2017: Designed a new course to bring theory and computational skills to undergraduate and graduate students. Electronic structure, Monte Carlo, and molecular dynamics simulations on chemical systems. Scientific writing and presentation.
3. Chemistry 5531, *Statistical Mechanics*, University of Colorado, 3 semesters. Spring 2013, Spring 2014, Spring 2015: Problem-based learning modules (PBL) and problem sets based on contemporary research in statistical mechanics, including molecular dynamics.

4. Chemistry 4581, *Physical Chemistry Lab I*, Chemistry 4591, *Physical Chemistry Lab II*, University of Colorado, 1 semester. Fall 2013: Wrote a new undergraduate computational lab using molecular dynamics simulations to compute diffusion constants of simple liquids as a function of temperature and density.
5. Chemistry 4511, *Physical Chemistry I*, University of Colorado, 2 semesters. Spring 2012, Fall 2014: PBL modules based on energy and economy, global energy consumption and biological reactions. Conceptual and formal treatment of thermodynamics.
6. Chemistry 5581, *Introduction to Quantum Chemistry*, University of Colorado, 3 semesters. Fall 2009, Fall 2010, Fall 2011: Extensive supplementary lecture notes. PBL and problem sets based on modern research, including molecular and nanoscale phenomena. Developed a section on solid-state electronic structure.
7. Chemistry 6401, *Seminar: Physical Chemistry*, University of Colorado, 2 semesters. Fall 2010, Spring 2011: Managed seminar series, one speaker per week for two semesters. Facilitated discussion each week between graduate students and speaker at one hour session per week.
8. Instructor, Methods of Computer Simulation in Chemical Physics, MIT, January 2004: Created a course for MIT's Independent Activities Period (IAP). Covered material in both molecular dynamics simulations and the Monte Carlo method.
9. Teaching Assistant, Undergraduate Statistical Mechanics, MIT, Spring 2000.
10. Teaching Assistant, Undergraduate Quantum Mechanics, MIT, Fall 1999.

Training
FTEP Workshop: "Teaching in a Nutshell," 1/2012.
FTEP Workshop: "Syllabus Design Workshop," 11/2011.

Funding

Current

Iron Pyrite 100: Investigation into an Electronically Frustrated 2-D Material with Technological Significance
Role: Co-PI $ 490,000 7/2014 – 06/2018
NSF DMR. Award Number 1410215.
Joint theoretical and experimental (with PI Conrad Stoldt at CU) study into the electronic, magnetic, and structural properties of iron sulfide nanostructures.

CAREER: SusChem: Multiscale Modeling for Fluid Separation Across Two-Dimensional Molecular Sieves and Student-Centered Course Reform
Role: PI $ 625,000 4/1/2015 – 3/31/2020
NSF CHE: Award Number 1455365.
Theoretical modeling and method development for fluid transport and separation using two-dimensional crystals. Problem-based learning course reform at both undergraduate and graduate levels.

Previous

A Theoretical Study of Coherent Energy Transport in Polymers
Role: PI $100,000 7/13–6/15
Petroleum Research Foundation (PRF) New Directions (ND).
Theoretical investigation of quantum coherent energy transfer pathways in polymers using the numerical renormalization group, theory of few-molecule vibrational dephasing dynamics, and triplet-triplet entanglement.

Gold Nanocrystal Therapeutics for the Treatment of Multi-drug Resistant Pathogens
Role: Co-PI $100,000 11/10–11/12
Bill and Melinda Gates Foundation

Joint theoretical and experimental (with PI Dan Feldheim at CU) study of nanoparticle therapeutics. Structure-function relationships for ligand-coated gold nanoparticles from theory and simulation.

Multiple Exciton Generation in Nanostructures: From Theory to Design
Role: PI $50,000 3/10–8/11
Center for Revolutionary Solar Photoconversion (CRSP)
Nonperturbative dynamics of photophysical process in carbon nanotubes from quantum field theory.

Service

Faculty search committee (2013–2014, 2015–2016).

Local organizer of the International Congress of Quantum Chemistry (2012).

Member of the Committee on Chemical Physics and Academic advisor (Chemistry) for the Ph. D. program in Chemical Physics (2012-current). Helped write rules and guidelines for the program in 2012.

Physical Chemistry representative to the Graduate Recruiting Committee (2009-2013, 2015).

Hosted and scheduled the Departmental "Summer Speaker," series of Colloquia (2010).

Served on Undergraduate Curriculum Committee (2010-2012).

Research Group Members

Graduate Students

Steven Strong — Joined 11/2012
B.S. Chemistry — Colorado School of Mines
Ph.D. candidate, Chemical Physics. Self-assembly of acene molecular crystallites. Atomistic hydrodynamics, method development and application to desalination.

Alyssa Landin — Joined 11/2013
B.S. Chemistry — Luther College
Ph.D. candidate, Chemical Physics. Magnetism, superconductivity and opto-electronic properties of iron pyrite and iron sulfide nanoparticles.

Peyton Cline — Joined 11/2015
B.S. Chemistry — Princeton University
Thermoelectric properties and self-assembly rules for perovskites.

Izzy Lattke — Joined 11/2015
B.S. Chemistry — Clark University
Colloidal analogs of active glass mixtures.

Alumni

Steven S. Strong (Ph.D., Chemical Physics, University of Colorado, Boulder 2012–2017. B.S. Colorado School of Mines).
Starting Postdoc with Jim Skinner at University of Chicago Jan. 2018.

Joe Ostrowski (Ph.D., Chemical Physics, University of Colorado, Boulder 2009–2014. B.S. University of Minnesota).
Currently faculty at Ridgewater College, Wilmar, MN.

Paul Teichen (Ph.D., Chemical Physics, University of Colorado, Boulder 2009–2015. B.S. Western Washington University).
Currently postdoc with Adam Willard at MIT, Cambridge, MA.

Kevin Pilkiewicz (Postdoc 2011–2014. Ph.D., Stanford. A.B., Harvard).
Currently Research Scientist at U.S. Army Corps of Engineers Environmental Laboratory, Vicksburg, MS.

Mark Sweeney (Postdoc 2011–2014. Ph.D., Colorado State University. B.S. Santa Clara State).
Currently Software Engineer Rogue Wave Software, Boulder CO.

Henri Hay (Master's Thesis Student, 2013. co-supervised with Université Pierre et Marie Curie).
Currently Ph.D. student at Université Pierre et Marie Curie, Paris, France.

Josh Kelley (Undergraduate, CU Physics, 2010).
Currently a physics graduate student, UCLA, Los Angeles, CA.

Dalee Zhou (Undergraduate, Amherst College Chemistry, 2010).
Currently enrolled in Cornell Medical School, New York, NY.