Thomas J. Lane

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ORCID:	0000-0003-2627-4432
GitHub:	github.com/tjlane
Nationality:	USA
Nickname:	"TJ"

Education

Stanford University, Stanford CA. PhD Chemistry, April 2015.
Thesis: "Modern theory of protein folding."

Pomona College, Claremont CA. BA Chemistry, May 2010.

Academic Positions

Group Leader, Deutsches Elektronen-Synchrotron "DESY" *Hamburg, DE. Aug/2020-present*
Leader: Photobiology Group. Center for FEL Science (CFEL).

Staff Scientist, SLAC Nat'l Accelerator Lab *Menlo Park, CA. Jan/2020-July/2020*
Machine learning group. Permanent academic position.

Associate Staff Scientist, SLAC Nat'l Accelerator Lab *Menlo Park, CA. June/2015-Jan/2020*
Linac coherent light source (LCLS). Tenure-track.

PhD Student, Stanford University *Stanford, CA. Sept/2010-Apr/2015*
Research group of Vijay Pande. Teaching & research.

Industry Positions

Principal Scientist, CHARM Therapeutics *Cambridge, UK. Nov/2022-May/2024*
Technical strategy & ML/experiment intersection.

Scholarship

Journal Publications:	70
Book Chapters:	1
Total Citations:	7700+
H-index:	35
PI role in project:	10
High Impact (Science or Nature):	6
Scholarly Grants & Awards:	11

→ https://scholar.google.com/citations?user=fWw8K2gAAAAJ&hl=en

Publications

Articles: First or Corresponding Author

* Indicates communicating authorship following PI role

19. * Stransky, M; **Lane, T. J.**; Gorel, A.; Boutet, S.; Schlichting, I.; Mancuso, A. P.; Jurek, Z.; Ziaja B. (2024). Ionization by XFEL radiation produces distinct structure in liquid water *Comms Phys* in press.

18. * Reinke, P. Y. A.; Schubert, R.; et. al.; **Lane, T. J.** (2024). SARS-CoV-2 M^{pro} responds to oxidation by forming disulfide and NOS/SONOS bonds. *Nat. Commun.* 15, 3827.

17. * Christou, N-E; Apostolopoulou, V; Melo, D. V. M.; et al.; **Lane, T. J.** (2023). Time-resolved crystallography captures light-driven DNA repair. *Science*, 382 (6674), 1015-1020.

16. * **Lane, T. J.** (2023). Protein structure prediction has reached the single-structure frontier. *Nat Methods*. DOI: 10.1038/s41592-022-01760-4.

15. * **Lane, T. J.**; Ratner, D. (2020). What are the advantages of ghost imaging? Multiplexing for x-ray and electron imaging. *Opt. Express*, 28 (5), 5898-5918.

14. * Barmherzig, D; Sun, J; Li, P-N; **Lane, T. J.** (2018). On Block-Reference Coherent Diffraction Imaging *Imaging and Applied Optics* 10.1364/COSI.2018.CTH1B.1.

13. * **Lane, T. J.** (2018). Biomolecular Imaging with Megavolt Electrons: Opportunities and Challenges for an Ultrafast Electron Microscope at SLAC. *SLAC SciDocs* SLAC-R-1093.

12. * Peck, A.; Poitevin, F., **Lane, T. J.** (2018). Intermolecular correlations are necessary to explain diffuse scattering from protein crystals. *IUCrJ* 5, 211-222.

11. * Shi, J.; Nobrega, R. P.; Schwantes, C.; Kathuria, S. V.; Bilsel, O.; Matthews, C. R.; **Lane, T. J.**; Pande, V. S. (2017). Atomistic structural ensemble refinement reveals non-native structure stabilizes a sub-millisecond folding intermediate of CheY. *Scientific Reports*, 1-13.

10. * Shi, L.; Wetzstein, G.; **Lane, T. J.** (2016). A Flexible Phase Retrieval Framework for Flux-limited Coherent X-Ray Imaging. *arXiv*:1606.01195v1.

9. **Lane, T. J.**; Schwantes, C. R.; Beauchamp, K. A.; Pande V. S. (2014) Efficient inference of protein structural ensembles *arXiv*:1408.0255.

8. **Lane, T. J.**; Schwantes, C. R.; Beauchamp, K. A.; Pande V. S. (2013) Probing the Origins of Two-State Folding *J. Chem. Phys.* 139, 145104.

7. **Lane, T. J.** and Pande V. S. (2013) Inferring the Rate-Length Law of Protein Folding. *PLoS ONE* DOI: 10.1371/journal.pone.0078606

6. **Lane, T. J.**; Shukla, D.; Beauchamp, K. A.; Pande V. S. (2013) To milliseconds and beyond: challenges in the simulation of protein folding *Curr. Op. Struct. Biol.* 23(1) 58-65.

5. **Lane, T. J.** and Pande V. S. (2013) Eigenvalues of the Homogeneous Finite Linear One Step Master Equation: Applications to Downhill Folding *J. Chem. Phys.* 6(12) 137, 215106.

4. **Lane, T. J.** and Pande, V. S. (2012) A Simple Model Predicts Experimental Folding Rates and a Hub-Like Topology *J. Phys. Chem. B* 116(23) 6764-6774.

3. **Lane, T. J.**; Bowman, G. R.; Beauchamp, K. A.; Voelz, V. A; Pande, V. S. (2011) Markov State Model Reveals Folding and Functional Dynamics in Ultra-Long Trajectories. *J. Am. Chem. Soc.* 133(45) 18413-18419.

2. **Lane, T. J.** et al. (2008) Dual-Beam Polarization Interferometry Resolves Mechanistic Aspects of Polyelectrolyte Adsorption. *Langmuir* 24(19) 10633-10636.

1. **Lane, T. J.** et al. (2008) Ultrasonic Rheology of the Aqueous Phase of SDS Micellar Systems. *Analyical Chemistry* 80(20), 7840-7845.

Articles: Co-authored

51. Peck, A; **Lane, T. J.**; F Poitevin (2023). Modeling diffuse scattering with simple, physically interpretable models. *Methods in enzymology* 688, 169-194.

50. Aithani, L. et al. (2023) Advancing structural biology through breakthroughs in AI. *Curr Op Struct Bio* 80, 102601.

49. Amann-Winkel, K. et al. (2023). Liquid-liquid phase separation in supercooled water from ultrafast heating of low-density amorphous ice. *Nat Commun* 14, 442.

48. Al-Haddad, A., et al. (2022). Observation of site-selective chemical bond changes via ultrafast chemical shifts. *Nat Commun*, 13, 7170.

47. Chitturi, S. R. et al (2022). A machine learning photon detection algorithm for coherent x-ray ultrafast fluctuation analysis. *Structural Dynamics*, 9, 054302.

46. Hammarström, B; **Lane, T. J.**; Batili, H.; Sierra, R.; Wiklund, M.; Sellberg, J. A. (2022). Acoustic Focusing of Protein Crystals for In-Line Monitoring and Up-Concentration during Serial Crystallography *Anal Chem*, online. 10.1021/acs.analchem.2c01701.

45. Adam, V. et al (2022). Rational Control of Off-State Heterogeneity in a Photoswitchable Fluorescent Protein Provides Switching Contrast Enhancement. *ChemPhysChem*, e202200192.

44. Srinivasan, V. et al (2022). Antiviral activity of natural phenolic compounds in complex at an allosteric site of SARS-CoV-2 papain-like protease. *Commun Biol* 5, 805.

43. Ladd-Parada, M. et al (2022). Following the Crystallization of Amorphous Ice after Ultrafast Laser Heating. *J Phys Chem B* 126 (11) 2299.

42. Esmaeildoost, N. et al (2021). Anomalous temperature dependence of the experimental x-ray structure factor of supercooled water. *J Chem Phys* 155 (21) 214501.

41. Sun, Y. et al (2021). Nonuniform Flow Dynamics Probed by Nanosecond X-Ray Speckle Visibility Spectroscopy. *Phys. Rev. Lett.* 127 (5) 058001.

40. Sorigue, D. et al (2021). Mechanism and dynamics of fatty acid photodecarboxylase. *Science*. 372 (6538), eabd5687

39. Günther, S.; Reinke, P., et al (2021). X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. *Science* 372 (6542) 642-646.

38. Yun, J.-H. et al (2021). Early-stage dynamics of chloride ion-pumping rhodopsin revealed by a femtosecond X-ray laser. *PNAS* 118 (13) e2020486118.

37. Pathak, H. et al (2021). Enhancement and maximum in the isobaric specific-heat capacity measurements of deeply supercooled water using ultrafast calorimetry. *PNAS* 118 (6) e2018379118.

36. Gruenbein, M. L. et al (2021). Observation of shock-induced protein crystal damage during megahertz serial femtosecond crystallography. *Phys. Rev. Research* 3, (1) 013046.

35. Coakley J. et al (2020). Femtosecond quantification of void evolution during rapid material failure. *Sci Advances* EABB4434.

34. Kim, K.-H.; Amann-Winkel, K. et. al. (2020). Experimental observation of the liquid-liquid transition in bulk supercooled water under pressure. *Science* 370 (6519) 978-982.

33. Kabra, K.; Li, S.; Cropp, F.; **Lane, T. J.**; Musumeci, P.; Ratner, D. (2020). Mapping Photocathode Quantum Efficiency with Ghost Imaging. arXiv:1910.11926.

32. Driver, T. et al (2020). Attosecond Transient Absorption Spooktroscopy: a ghost imaging approach to ultrafast absorption spectroscopy. *Phys. Chem. Chem. Phys.* DOI: 10.1039/c9cp03951a.

31. Stankus, B. et al (2019). Ultrafast X-ray scattering reveals vibrational coherence following Rydberg excitation. *Nat Chem*, 11, 716-721.

30. Lieske, J. et al (2019). On-chip crystallization for serial crystallography experiments and on-chip ligand-binding studies. *IUCrJ*, 6(4), 714-728.

29. Barmherzig, D; Sun, J.; Li, P-N; **Lane, T. J.** and Candes, E. J (2019). Holographic Phase Retrieval and Reference Design. *Inverse Problems*, IP-102044.R1.

28. Ratner, D.; Cryan, J. P.; **Lane, T. J.**; Li, S.; Stupakov, G. (2019). Pump-Probe Ghost Imaging with SASE FELs. *Phys Rev X*, 9, 011045

27. Ruddock, J. et al (2019). Simplicity beneath Complexity: Counting Molecular Electrons Reveals Transients and Kinetics of Photodissociation Reactions. *Angew Chem*, 58(10), 371-6375

26. Sierra, R. G.; Batyuk, A.; Sun, Z.; Aquila, A.; Hunter, M. S.; **Lane, T. J.**; M Liang, M. et al. (2019). The Macromolecular Femtosecond Crystallography Instrument at the Linac Coherent Light Source. *J Synch Rad*. 26(2), 346-357.

25. Barmherzig, D; Sun, J; Candes, E. J.; **Lane, T. J.** and Li, P-N (2019). Dual-Reference Design for Holographic Coherent Diffraction Imaging. arXiv:1902.02492.

24. Barmherzig, D; Sun, J; Candes, E. J.; **Lane, T. J.** and Li, P-N (2019). Holographic Phase Retrieval and Optimal Reference Design. arXiv:1901.06453.

23. Yong, H. et al. (2018). Determining Orientations of Optical Transition Dipole Moments Using Ultrafast X-ray Scattering. *J Phys Chem Lett*, 9(22), 6556-6562.

22. S. Li; F. Cropp; K. Kabra; **Lane, T. J.**; Weitzstein, G; Musumeci, P.; Ratner, D. (2018). Electron ghost imaging. *Phys Rev Lett* 121(11), 114801.

21. Nogly et al. (2018). Retinal isomerization in bacteriorhodopsin captured by a femtosecond x-ray laser. *Science* 361, 194 (eaat0094).

20. Perakis, F; Camisasca, G; **Lane, T. J.**; et al (2018). Coherent x-rays reveal the influence of cage effects on ultrafast water dynamics. *Nat Comm* 9, 1917.

19. Shen, X.; Li, R. K.; Lundström, U.; **Lane, T. J.**; Reid, A. H.; Weathersby, S. P.; Wang, X. J. (2017). Femtosecond mega-electron-volt electron microdiffraction. *Ultramicroscopy* 184PA, 172-176.

18. Coquelle et al. (2018). Chromophore twisting in the excited state of a photoswitchable fluorescent protein captured by time-resolved serial femtosecond crystallography. *Nat Chem* 10(1), 31-37.

17. Herrmann, J.; et al. (2017). Environmental Calcium Controls Alternate Physical States of the Caulobacter Surface Layer. *Biophys. J.* 112, 1841-1851.

16. Thayer, J., Damiani, D., Ford, C., Dubrovin, M., Gaponenko, I., O'Grady, C. P., et al. (2017). Data systems for the Linac coherent light source. *Adv. Struct. Chem. Imag.*, 1-13.

15. Stankus, B.; Budarz, J. M.; Kirrander, A.; Rogers, D.; Robinson, J.; **Lane, T. J.**; et al. (2016). Femtosecond photodissociation dynamics of 1,4-diiodobenzene by gas-phase X-ray scattering and photoelectron spectroscopy. *Faraday Discussions*, 194, 525-536.

14. Young, I. D; et al. (2016). Structure of photosystem II and substrate binding at room temperature. *Nature* 540, 453-457.

13. Mendez, D.; et al. (2016). Angular correlations of photons from solution diffraction at a free-electron laser encode molecular structure. *IUCrJ* 3, 420-429.

12. Hunter, M. S.; et al. (2016). Selenium single-wavelength anomalous diffraction de novo phasing using an X-ray Free Electron Laser. *Nat. Comm*, 7, 13388.

11. Stan, C. A., Milathianaki, D., Laksmono, H., Sierra, R. G., McQueen, T. A., Messerschmidt, M., Williams, G. J.; Koglin, J. E.; **Lane, T. J.**; et al. (2016). Liquid explosions induced by X-ray laser pulses. *Nat. Phys.*, 1-7.

10. Damiani, D.; Dubrovin, M.; Gaponenko, I.; Kroeger, W.; **Lane, T. J.**; Mitra, A.; O'Grady, C.P.; Salnikov, A.; Sanchez-Gonzalez, A.; Schneider, D.; Yoon C.H.; (2016) Linac Coherent Light Source data analysis using psana. *J. Appl. Cryst.* 49, 672-679.

9. Mariani, V.; Morgan, A., Yoon, C. H.; **Lane, T. J.**; White, T. A.; O'Grady, C., et al. (2016). OnDA: online data analysis and feedback for serial X-ray imaging. *J. Appl. Cryst.* 49, 1-8.

8. Minitti, M. P.; Budarz, J. M.; Kirrander, A.; Robinson, J. S.; Ratner, D.; **Lane, T. J.**; Zhu, D.; Glownia, J.M.; Kozina, M.; Lemke, H. T.; Sikorski, M.; Feng, Y.; Nelson S.; Saita, K.; Stankus B.; Northey T.; Hastings, J. B.; Weber, P. M. (2015) Imaging Molecular Motion: Femtosecond X-Ray Scattering of an Electrocyclic Chemical Reaction *Phys. Rev. Lett.* 114, 255501.

7. McGibbon, R. T.; Beauchamp, K. A.; Schwantes, C. R.; Wang, L.-P.; Hernandez, C. X.; Harrigan, M. P.; **Lane, T. J.**; Swails, J. M.; Pande, V. S. (2015) MDTraj: a modern, open library for the analysis of molecular dynamics trajectories. *Biophysical J.* 109(8), 1528-1532

6. Mendez, D.; **Lane, T. J.**; et. al. (2014) Observation of correlated X-ray scattering at atomic resolution *Phil. Trans. Royal Soc. B* 369, 20130315.

5. Eastman, P.; Friedrichs, M. S.; Chodera, J. C.; Radmer, R. J.; Bruns, C. M.; Ku, J. P.; Beauchamp, K. A.; **Lane, T. J.**; Wang, L.-P.; Shukla, D.; Tye, T; Houston, M.; Stich, T.; Klein, C.; Shirts, M. R.; Pande V. S. (2013) OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation *J. Chem. Theory Comput.*, 9(1) 461-469.

4. Beauchamp, K. A.; Bowman, G. R.; **Lane, T. J.**; Maibaum, L.; Haque, I. S.; Pande, V. S. (2011) MSMBuilder2: Modeling Conformational Dynamics on the Picosecond to Millisecond Scale. *J. Chem. Theory Comput.* 7(10) 3412-3419.

3. Frau, A. F.; **Lane, T. J.**; Schlather, A. E.; Park, J. Y.; Advincula, R. C. (2011) Modulating Electrochemical Activity in Polyaniline/Titanium Oxide Hybrid Nanostructured Ultrathin Films. *Ind. Eng. Chem. Res.* 50(9) 5532-5542.

2. Zwang, T. J.; Fletcher, W. R.; **Lane, T. J.**; Johal, M. S. (2009) Characterization of the Layer of Hydration of a Supported Lipid Bilayer. *Langmuir* 26(7) 4598-4601.

1. Kett, P.; Casford, M.; Yang, A.; Johal, M.; **Lane, T. J.**; Davies, P. (2008) Structural Changes in a Polyelectrolyte Multilayer Assembly Investigated by Reflection Absorption Infrared Spectroscopy and Sum Frequency Generation Spectroscopy. *J. Phys. Chem. B* 113(6) 1559-1568.

Book Chapters

Ultrasonic Rheology of Mixed-Phase Systems: Using a QCM as an Effective Rheological Device: Theory and Applications for Combined Surface and Bulk Rheology. **Thomas J. Lane**. *Amphiphiles: Molecular Assembly and Applications.* Ed. Ramanathan Nagarajan. Chapter 10, pp 145-174.

Grants, Awards, Honors

Royal Society of Chemistry Horizon Award: Ultrafast X-ray Scattering (2021).

Faculty, International Max Planck Research School for Ultrafast Imaging & Structural Dynamics (2021).

Member, DFG Excellence Cluster on Advanced Imaging of Matter "AIM" (2020).

Helmholtz Young Investigator Group Leader Award, 1.8M EUR (2020-2026).

DoE SciDAC: Designing Photocatalysts Through Scalable Quantum Mechanics and Dynamics. Principle author with T. Martinez, $4M. Managed 4-PI photocatalyst design team (2017-2020).

NSF Graduate Research Fellowship (2010-2013)

John Stauffer Academic Award (2010)

The Frank Parkhurst Brackett, Jr. and David Wark Brackett Prize (2010)

Wig Grant for Curriculum Development (2010)

Barry M. Goldwater Scholarship (2009)

Beckman Scholarship (2008)

Invited Talks

Time-resolved crystallography captures light-driven DNA repair. UK XFEL Meeting. Royal Society, London (2024).

Time-resolved crystallography captures light-driven DNA repair. 7th Ringberg Workshop on Structural Biology. Tegernsee (2024).

Statistical crystallography reveals correlated motions of SARS-CoV-2 Mpro. CFEL retreat, Timmendorf (2022).

Can we witness proteins traversing conical intersections via FEL-based crystallography? Imaging European Crystallographic Meeting, Versailles (2022).

Statistical crystallography reveals correlated motions of SARS-CoV-2 Mpro. Pacifichem (online). (2021).

Statistical crystallography reveals correlated motions of SARS-CoV-2 Mpro. Helmholtz: Mater, Materials, Life (MML) (online). (2021).

Revealing allosteric pathways via large-scale crystallographic studies. BioXFEL (online). (2021).

The quest for correlated motion in proteins: progress through diffuse scatter and multi-crystal analysis. UHH Hamburg. (2020).

What Can We Learn from Diffuse Scatter? Applied Physics Seminar. KTH Stockholm. (2019).

Putting the Femtosecond in SFX: Ultrafast Crystallography. Pittsburg Diffraction Meeting. (2018).

What Can We Learn from Diffuse Scatter? 5th Ringberg Conference on XFELs in Biology. (2018).

Phase Retrieval with Prior Information. LCLS/SSRL User's Meeting. Menlo Park, CA. (2016).

Protein Evolution and Design: Session Chair. Protein Folding GRC, Galveston, TX. (2014)

Boltzmann Takes On Biology: The Next Frontier in Structure. Chemistry Colloquium, Pomona College, CA (2013)

Transition State Ensembles: The View from Simulation and Experiment. Protein Folding Consortium, Stony Brook, NY. (2012)

To the Exa-Scale and Beyond: Statistically Motivated Linear Scaling for Protein Dynamics. Titan Summit, Oak Ridge, TN. (2011)

Markov State Model Reveals Folding and Functional Dynamics in Ultra-Long Trajectories. Biophysics Symposium, Stanford, CA. (2010)

Ultrasonic Rheology of Mixed-Phase Systems. Amgen, Thousand Oaks, CA. (2010)

Ultrasonic Rheology of Surfactant Systems. Biolin Scientific Surface Science Symposium, Pomona College, CA. (2010)

Ultrasonic Rheology of SDS Microemulsions. Presented orally at Stanford's QCM-D User's Meeting. *Best Presentation Award* (2007)

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