ELLEN D. ZHONG

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EDUCATION AND EXPERIENCE

 2022 - present Princeton University, Princeton, NJ. Assistant Professor, Department of Computer Science Associated Faculty: Center for Statistics and Machine Learning, Omenn-Darling Bioengineering Institute, Quantitative and Computational Biology, Princeton Language Initiative
 2017 - 2022 Massachusetts Institute of Technology, Cambridge, MA. Ph.D. Computational and Systems Biology, Computer Science and Artificial Intelligence Laboratory

> Advisors: Bonnie Berger, Joseph H. Davis Thesis: "Machine learning for reconstructing dynamic protein structure from cryo-EM images"

2010 - 2014 University of Virginia, Charlottesville, VA.
 B.S. Chemical Engineering with highest distinction
 Advisor: Michael R. Shirts
 Thesis: "Thermodynamics of protein folding with Hamiltonian Monte Carlo simulations"

OTHER PROFESSIONAL EXPERIENCE

2023 - present	Chan Zuckerberg Imaging Institute, Scientific Advisory Board
2023 - present	Deep Apple Therapeutics, Scientific Advisory Board
2022 - present	Flatiron Institute, Visiting Researcher
Summer 2021	Google DeepMind, Research Scientist Intern Hosted by John Jumper and the AlphaFold team
2014 - 2017	D. E. Shaw Research, Scientific Programmer Algorithms and infrastructure for free energy calculations
Summer 2013	D. E. Shaw Research, Scientific Programmer Intern
Summer 2011	NASA/Johns Hopkins Applied Physics Lab MESSENGER Imaging Team

PUBLICATIONS (*Co-corresponding, +Equal contribution)

- Deep reconstructing generative networks for visualizing dynamic biomolecules inside cells. Rangan R⁺, Feathers R⁺, Khavnekar S, Lerer A, Johnston J, Kelley R, Obr M, Kotecha A^{*}, Zhong ED^{*}. Nature Methods, 2024.
- 2. Revealing biomolecular structure and motion with neural *ab initio* cryo-EM reconstruction. Levy A, Poitevin F, Johnston J, Vallese F, Clarke OB, Wetzstein G, **Zhong ED**. *bioRxiv*, 2024.
- 3. Solving Inverse Problems in Protein Space Using Diffusion-Based Priors. Levy A, Chan ER, Fridovich-Keil S, Poitevin F, **Zhong ED**, Wetzstein G. *arXiv*, 2024.
- 4. Accurate structure prediction of biomolecular interactions with AlphaFold 3. Abramson J, Adler J, Dunger J, ..., **Zhong ED**, ..., Jaderberg M, Hassabis D, Jumper JH. *Nature*, *2024*.
- 5. Cryo-ET reveals the in situ architecture of the polar tube invasion apparatus from microsporidian parasites. Usmani M, Coudray N, Riggi M, Raghu R, Ramchandani H, Bode D, Kopylov M, **Zhong ED**, Iwasa JH, Ekiert DC, Bhabha G. *bioRxiv*, 2024.
- Conformational states of the microtubule nucleator, the γ-tubulin ring complex. Romer R, Travis SM, Mahon BP, McManus CT, Jeffrey PD, Coudray N, Raghu R, Rale MJ, Zhong ED, Bhabha G, and Petry S. *bioRxiv*, 2023.
- 7. Time-resolved cryo-EM (TR-EM) analysis of substrate polyubiquitination by the RING E3 anaphasepromoting complex/cyclosome (APC/C). Bodrug T, ... **Zhong ED**, Haselbach H, Brown NG. *Nature Structural and Molecular Biology*, 2023.
- 8. Conformational heterogeneity and probability distributions from single particle cryo-electron microscopy. Tang WS, **Zhong ED**, Hanson SM, Theide EH, Cossio P. *Current Opinion in Structural Biology*, 2023.
- 9. Amortized inference for heterogeneous reconstruction in cryo-EM. Levy A, Wetzstein G, Martel J, Poitevin F, **Zhong ED**. *Neural Information Processing Systems (NeurIPS)*, 2022.
- 10. Latent Space Diffusion Models of Cryo-EM Structures. Kreis K, Dockhorn T, Li Z, **Zhong ED**. *NeurIPS Machine Learning in Structural Biology (MLSB) Workshop*, 2022. Oral presentation.
- 11. Deep Generative Modeling for Volume Reconstruction in Cryo-Electron Microscopy. Donnat C, Levy A, Poitevin F, **Zhong ED**, Miolane N. *Journal of Structural Biology*, 2022.
- 12. Uncovering structural ensembles from single particle cryo-EM data using cryoDRGN. Kinman LF⁺, Powell BM⁺, **Zhong ED**^{*+}, Berger B^{*}, Davis JH^{*}. *Nature Protocols*, 2022.
- 13. Conformational landscape of the yeast SAGA complex as revealed by cryo-EM. Vasyliuk D, Felt J, **Zhong ED**, Berger B, Davis JH, Yip CK. *Scientific Reports*, 2022.
- 14. Cryo-EM structure of the plant 26S proteasome. Kandolf S, Grishkovskaya I, Belai K, Bolhuis DL, Amann S, Foster B, Imre R, Mechtler K, Schleiffer A, Tagare HD, **Zhong ED**, Meinhart A, Brown NG, Haselbach D. *Plant Communications*, 2022.
- CryoDRGN2: Ab initio neural reconstruction of 3D protein structures from real cryo-EM images.
 Zhong ED, Lerer A, Davis JH, Berger B. International Conference on Computer Vision (ICCV), 2021.
- 16. CryoDRGN: Reconstruction of heterogeneous cryo-EM structures using neural networks. **Zhong ED**, Bepler T, Berger B, Davis JH. *Nature Methods*, 2021.
- 17. Learning the language of viral evolution and escape. Hie B, **Zhong ED**, Berger B, Bryson B. Science, 2021

- 18. Structures of radial spokes and associated complexes important for ciliary motility. Gui M, Ma M, Sze-Tu E, Wang X, Koh F, **Zhong ED**, Berger B, Davis JH, Dutcher S, Zhang R, Brown A. *Nature Structural and Molecular Biology*, 2021.
- Exploring generative atomic models in cryo-EM reconstruction. Zhong ED, Lerer A, Davis JH, Berger B. NeurIPS Machine Learning in Structural Biology (MLSB) Workshop, 2020.
- 20. Learning mutational semantics. Hie B, **Zhong ED**, Bryson B, Berger B. *Neural Information Processing Systems (NeurIPS)* 2020.
- 21. RNA timestamps identify the age of single molecules in RNA sequencing. Rodriques SG, Chen LM, Liu S, **Zhong ED**, Scherrer JR, Boyden ES, Chen F. *Nature Biotechnology*, 2020.
- Reconstructing continuous distributions of 3D protein structure from cryo-EM images. Zhong ED, Bepler T, Davis JH, Berger B. International Conference on Learning Representations (ICLR) 2020. Spotlight presentation. Machine Learning in Computational Biology (MLCB), 2019. Oral presentation. NeurIPS Learning Meaningful Representations of Life (LMRL) workshop, 2019.
- 23. Explicitly disentangling image content from translation and rotation with spatial-VAE. Bepler T, **Zhong ED**, Kelley K, Brignole E, Berger B. *Neural Information Processing Systems (NeurIPS)* 2019.
- 24. Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. Shirts MR, Klein C, Swails JM, Yin J, Gilson MK, Mobley DL, Case DA, **Zhong ED**. J. Comput. Aid. Mol. Des. 2016.
- 25. Thermodynamics of Coupled Protein Adsorption and Stability using Hybrid Monte Carlo simulations. **Zhong ED**, Shirts MR. *Langmuir* 2014.
- 26. Areas of permanent shadow in Mercurys south polar region ascertained by MESSENGER orbital imaging. Chabot NL, Ernst CM, Denevi BW, ... **Zhong ED**. *Geophys. Res. Lett.* 2012.

TALKS AND PRESENTATIONS

2024:

- 1. Aug 2024: EMBO Practical Course on Advances in Cryo-EM Processing, Heidelberg, Germany
- 2. Aug 2024: 15th K.H. Kuo International Symposium on Cryo-EM Technology, Shenzhen, China
- 3. July 2024: AI for All Guest Lecture, Princeton, NJ
- 4. June 2024: Keynote, 3DEM Gordon Research Seminar, Castelldefels, Spain
- 5. June 2024: CVPR Workshop on Computer Vision for the Physical Sciences, Seattle, WA
- 6. June 2024: AI=Science: Strengthening the Bond Between the Sciences and Artificial Intelligence, Simons Institute, Berkeley, CA
- 7. May 2024: Cryo-ET Course at Monash, Virtual
- 8. May 2024: Omenn-Darling Bioengineering Institute Dedication, Princeton, NJ
- 9. May 2024: CCP-EM Spring Symposium, Nottingham, UK
- 10. Apr 2024: MIT 6.8710: Deep Learning in the Life Sciences Guest Lecture, Cambridge, MA
- 11. Apr 2024: Princeton CSML Seminar Series, Princeton, NJ
- 12. Mar 2024: EMBO|EMBL Symposium on AI and Biology, Heidelberg, Germany
- 13. Mar 2024: MPI Biophysics, Frankfurt, Germany
- 14. Jan 2024: EMBL Cryo-EM in Industry and Academia, Virtual

2023:

- 15. Dec 2023: NeurIPS Deep Learning and Inverse Problems Workshop, New Orleans, LA
- 16. Dec 2023: NeurIPS Generative AI and Biology Workshop, New Orleans, LA

- 17. Nov 2023: Toronto Vision Seminar, Toronto, Canada
- 18. Oct 2023: NYU Langone, New York, NY
- 19. Oct 2023: Keynote, CryoNet, Stockholm, Sweden
- 20. Sept 2023: MIT Bioinformatics Seminar, Cambridge, MA
- 21. Aug 2023: University of Copenhagen NNF Center for Protein Research, Copenhagen, Denmark
- 22. July 2023: American Crystallography Association Annual Meeting, Baltimore, MD
- 23. July 2023: Symposium on Geometry Processing, Genoa, Italy
- 24. June 2023: EMBL Heidelberg, Heidelberg, Germany
- 25. June 2023: Google Research, Virtual
- 26. June 2023: Flatiron Institute workshop on Cryo-EM methods, New York, NY
- 27. May 2023: University of Pennsylvania Structural Biology Symposium, Philadelphia, PA
- 28. May 2023: Princeton Catalysis Initiative, Princeton, NJ
- 29. May 2023: University of Michigan Cryo-EM Data Processing Workshop, Ann Arbor, MI
- 30. May 2023: ICLR Neural Fields Across Fields Workshop, Kigali, Rwanda
- 31. Apr 2023: UC Davis Department of Molecular and Cellular Biology, Davis, CA
- 32. Apr 2023: Stanford SCIEN Seminar Series, Palo Alto, CA
- 33. Apr 2023: Caltech Al4Science Seminar Series, Pasadena, CA
- 34. Mar 2023: University of Washington Institute of Protein Design, Seattle, WA
- 35. Mar 2023: North Atlantic Microscopy Society Annual Meeting, Princeton, NJ
- 36. Mar 2023: Columbia Physiology and Cellular Biophysics, New York, NY
- 37. Feb 2023: Biophysical Society Annual Meeting, San Diego, CA
- 38. Jan 2023: Brigham Young University Department of Chemistry and Biochemistry, Provo, UT **2022**:
- 39. Dec 2022: MIT 6.S980 Machine Learning for Inverse Graphics guest lecture, Cambridge, MA
- 40. Nov 2022: Institute of Pure and Applied Mathematics (IPAM) workshop, Los Angeles, CA
- 41. Nov 2022: Cold Springs Harbor Laboratory, Course on Cryo-EM, Long Island, NY
- 42. Nov 2022: Flatiron Institute Workshop on Sampling, Diffusion, and Transport, New York, NY
- 43. Nov 2022: Chan Zuckerberg Imaging Institute, Frontiers in Cryo-ET, San Francisco, CA
- 44. Oct 2022: Yale Department of Statistics and Data Science, New Haven, CT
- 45. Oct 2022: Keynote, MIT Molecule Machine Learning Conference, Cambridge, MA
- 46. Oct 2022: Purdue Department of Computer Science, Virtual
- 47. Oct 2022: Rutgers Institute for Quantitative Biomedicine and RCSB Protein Data Bank, Virtual
- 48. Sept 2022: Nature Conferences, Electron Microscopy for Physical and Life Sciences, Princeton, NJ
- 49. Sept 2022: Van Andel Institute, Virtual
- 50. Aug 2022: Microscopy & Microanalysis, Portland, OR
- 51. Jun 2022: CVPR, Neural Fields in Computer Vision Tutorial, New Orleans, LA
- 52. Apr 2022: ICLR Deep Generative Models for Highly Structured Data Workshop, Virtual
- 53. Apr 2022: VIB-VUB Center of Structural Biology, Virtual
- 54. Apr 2022: CCP-EM/CCPBioSim Cryo-EM Dynamics Discussion Meeting, Virtual
- 55. Mar 2022: Vienna Biocenter IMBA/IMP Young Investigator Symposium, Virtual
- 56. Mar 2022: SIAM Conference on Imaging Science, Cryo-EM Mini-symposium, Virtual
- 57. Mar 2022: SLAC/Stanford University, Palo Alto, CA

- 58. Mar 2022: John Hopkins University Cryo-EM Seminar Series, Virtual
- 59. Mar 2022: Brookhaven National Lab Applied Mathematics Seminar Series, Virtual
- 60. Mar 2022: International Conference on Image Analysis in Three-dimensional Cryo-EM, Lake Tahoe, CA
- 61. Mar 2022: OpenEye CUP Conference, Santa Fe, NM
- 62. Feb 2022: Princeton Department of Computer Science, Princeton, NJ
- 63. Feb 2022: Columbia Department of Computer Science, Virtual

2021:

- 64. Nov 2021: MRC Laboratory of Molecular Biology, Cambridge, UK
- 65. Nov 2021: The Francis Crick Institute, London, UK
- 66. Nov 2021: Microsoft Research New England, Virtual
- 67. Oct 2021: Session chair, 3DEM Gordon Research Conference, Waterville Valley, NH Cryo-EM and AlphaFold in translational research
- 68. Sept 2021: Stanford SLAC Users Meeting, Virtual
- 69. Aug 2021: RosettaCon, Virtual
- 70. Aug 2021: American Crystallographic Association Annual Meeting, Virtual
- 71. Apr 2021: CCP-EM Spring Symposium, Virtual
- 72. Apr 2021: GlaxoSmithKline (GSK), Virtual
- 73. Feb 2021: Princeton University Applied Mathematics IDeAS Seminar, Virtual
- 74. Feb 2021: UIUC Coordinated Science Laboratory Student Conference (CSLSC), Virtual

2020 and earlier:

- 75. Nov 2020: Vienna BioCenter, Research Institute of Molecular Pathology Seminar Series, Virtual
- 76. Sept 2020: SciLifeLab Advanced Cryo-EM Seminar Series, Virtual
- 77. Aug 2020: Microscopy & Microanalysis, Virtual
- 78. May 2020: SBGrid Annual Symposium, Virtual
- 79. Feb 2020: Relay Therapeutics, Cambridge, MA
- 80. Dec 2019: Machine learning in Computational Biology workshop, Vancouver, BC
- 81. Dec 2019: Poster: NeurIPS Learning Meaningful Representations of Life workshop, Vancouver, BC
- 82. Dec 2019: Harvard Cryo-EM Club, Cambridge, MA
- 83. Nov 2019: Poster: Janelia Women in Computational Biology Meeting, Ashburn, VA
- 84. Oct 2019: New England CryoEM symposium, Worchester, MA
- 85. Aug 2019: Poster: Flatiron Institute Computational Cryo-EM Workshop, New York, NY
- 86. Nov 2015: Out in STEM National Conference, Pittsburgh, PA

From silicon to medicine: Challenges in molecular dynamics for early-stage drug discovery

- 87. Oct 2015: Grace Hopper Annual Conference, Houston, TX
 - Optimizing molecular visualization for drug discovery.
- 88. Nov 2013: AIChE Annual Meeting, San Francisco, CA

Efficient simulation of protein stability on surfaces using a Hamiltonian Monte Carlo approach.

TEACHING

Fall 2024	COS 302: Mathematics for Machine Learning
Spring 2024	COS IW10: Molecular Machine Learning
Fall 2023	COS 597N: Machine Learning for Structural Biology
Fall 2022	COS 597N: Machine Learning for Structural Biology

MENTORING

Postdoctoral Fellows

2023-Present	Ryan Feathers, Co-advised with Fred Hughson (MOL), Princeton Presidential
	Postdoctoral Fellow
2023-2024	Ramya Rangan, Now Atomic Al
Graduate Studen	ts
2023-Present	Minkyu Jeon, Ph.D. Computer Science
2023-Present	Alkin Każ, Ph.D. Computer Science, M.Eng. Electrical and Computer Engineering,
2022-Present	Rishwanth Raghu, Ph.D. Computer Science, M.S. Computer Science
2022-2023	Mark Castellano, M.Eng. Electrical and Computer Engineering
Undergraduate S	tudents
2024-Present	Cloris Cheng, B.S. Computer Science (Caltech)
2024-Present	Adele Peng, A.B. Chemistry
2023-2024	David Shustin, B.S. Computer Science, Kephart '80 Prize in Engineering Physics
2023-2024	Vicky Feng, A.B. Computer Science, Senior Thesis Prize
Other Group Men	nbers

2023-Present	Michal Grazdowski, Senior Research Software Engineer
2022-2023	Vineet Bansal, Visiting Research Software Engineer

ACADEMIC SERVICE

Area chair:	Neural Informational Processing Systems (NeurIPS)
Reviewer:	Nature, Science, Nature Methods, Neural Information Processing Systems (NeurIPS),
	International Conference on Learning Representations (ICLR), International Conference
	on Machine Learning (ICML), Machine Learning in Computational Biology Workshop
	(MLCB), Machine Learning in Structural Biology Workshop (MLSB), IEEE Transactions on
	Computational Biology and Bioinformatics, IEEE Transactions on Computational
	Imaging, Biophysical Journal, Journal of Physical Chemistry Letters, IUCrJ, Scientific
	Reports
Meetings:	Organizer, 2024 Nature Conferences, Frontiers in Electron Microscopy for Physical and
	Life Sciences
	Organizer, 2023 Machine Learning in Structural Biology Workshop at NeurIPS
	Organizer, 2022 Machine Learning in Structural Biology Workshop at NeurIPS
	Organizer, 2021 Machine Learning in Structural Biology Workshop at NeurIPS
	Organizer, 2020 Machine Learning in Structural Biology Workshop at NeurIPS

AWARDS

Fall 2023	Teaching Award, Princeton SEAS
2021	American Crystallographic Association Etter Student Lecturer Award
2019	Best paper award at Machine Learning in Computational Biology Workshop
Spring 2018	Teaching Award, MIT Biology
2017	NSF Graduate Research Fellowship
2014	NSF Graduate Research Fellowship (Declined)
2014	Louis T. Rader Chemical Engineering Prize
2014	American Institute of Chemists Award
2013	Barry M. Goldwater Scholarship
2012, 2013	Astronaut Scholarship

PRESS

07/2024	Quanta Magazine, "How AI Revolutionized Protein Science but Didn't End It"
11/2023	BitesizeBio webinar, "Machine Learning Approach to Cellular Cryo-Tomography"
10/2023	The Atlantic Festival, Panelist "What Would It Take to Transform Drug Discovery With
	<u>AI?"</u>
06/2023	Princeton University News, <u>"Princeton's 5th PCI Symposium"</u>
06/2023	Webinar interview with the Hive Think Tank, "Beyond Language: Reasoning over Non-
	Language Data with Generative AI"
09/2022	Video podcast interview on the Plunge, Thermo Fisher
09/2021	VPRO TV Documentary, <u>"Tomorrow's medicine"</u>
06/2021	MIT News, <u>"The power of two"</u>