

ELLEN D. ZHONG

zhonge@mit.edu ◊ people.csail.mit.edu/zhonge

EDUCATION

- Massachusetts Institute of Technology** 2017 - Present
Ph.D. Student, Computational and Systems Biology
Areas of concentration: Machine learning, cryo-EM, structural biology, computational biology
- University of Virginia** 2010 - 2014
B.S. Chemical Engineering with highest distinction (GPA: 3.96/4.0)
Areas of concentration: Statistical mechanics, protein folding

RESEARCH AND WORK EXPERIENCE

- DeepMind**, London, UK Summer 2021
Research Scientist Intern - Science team
Hosted by John Jumper and the AlphaFold team
- MIT Computer Science and Artificial Intelligence Lab**, Cambridge, MA 2017 - Present
Advisors: Prof. Bonnie Berger (Mathematics, EECS), Prof. Joseph H. Davis (Biology)
Machine learning algorithms for 3D reconstruction of protein structures from cryo-electron microscopy images.
- D. E. Shaw Research**, New York, NY 2014 - 2017
Scientific Programmer
Algorithms and infrastructure for estimating protein-drug binding free energy calculations from molecular dynamics simulation on Anton supercomputers.
Automated tools for ligand forcefield fitting via *ab initio* quantum mechanical calculations.
- University of Virginia**, Charlottesville, VA 2011 - 2014
Advisor: Prof. Michael R. Shirts (Chemical Engineering)
Hamiltonian Monte Carlo simulations for estimating protein-folding thermodynamics.
- D. E. Shaw Research**, New York, NY Summer 2013
Scientific Programmer Intern
Production-scale workflow for calculating binding free energies of small molecules to cryptic protein pockets identified via molecular dynamics simulations.
- NASA/Johns Hopkins University Applied Physics Lab**, Laurel, Maryland Summer 2011
MESSENGER Imaging Team Intern
Analysis software for the MESSENGER south polar imaging campaign to investigate the existence of ice in Mercurius impact craters.

JOURNAL PUBLICATIONS

- CryoDRGN: Reconstruction of heterogeneous cryo-EM structures using neural networks.
Zhong ED, Beppler T, Berger B, Davis JH.
Nature Methods, 2021. doi:10.1038/s41592-020-01049-4.
- Learning the language of viral evolution and escape.
Hie B, **Zhong ED**, Berger B, Bryson B.
Science, 2021. doi:10.1126/science.abd7331.
- RNA timestamps identify the age of single molecules in RNA sequencing.
Rodrigues SG, Chen LM, Liu S, **Zhong ED**, Scherrer JR, Boyden ES, Chen F.
Nature Biotechnology, 2020. doi:10.1038/s41587-020-0704-z.

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, 2020. <https://doi.org/10.1038/s41594-020-00530-0>.

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. Aided. Mol. Des. 2016. doi:10.1007/s10822-016-9977-1.

Thermodynamics of Coupled Protein Adsorption and Stability using Hybrid Monte Carlo simulations.

Zhong ED, Shirts MR.

Langmuir 2014. doi:10.1021/la500511p

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. doi:10.1029/2012GL051526.

CONFERENCE AND WORKSHOP PUBLICATIONS

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.

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.

Learning mutational semantics.

Hie B, **Zhong ED**, Bryson B, Berger B.

Neural Information Processing Systems (NeurIPS) 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.

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.

SELECTED PRESENTATIONS

CryoDRGN: Reconstructing continuous distributions of protein structure from cryo-EM images.

- Invited talk: Deep Generative Models for Highly Structured Data Workshop (tentative) at ICLR, April, 2022
- Invited talk: SIAM Conference on Imaging Science, Cryo-EM Mini-symposium, Berlin, Germany, March, 2022
- Invited talk: International Conference on Image Analysis in Three-dimensional Cryo-EM, Lake Tahoe, CA, March, 2022
- Invited talk: MRC Laboratory of Molecular Biology, Cambridge, UK, November, 2021
- Discussion Leader: Gordon Research Conference, Visualizing Biological Complexity Across Scales, October, 2021

- Poster: Gordon Research Seminar, Visualizing Biological Complexity Across Scales, October, 2021
- Invited talk: Scientific Computing in Structural Biology Workshop, Stanford SLAC Users Meeting, September, 2021
- Invited talk: RosettaCon, August, 2021
- Invited talk: American Crystallographic Association Annual Meeting, August, 2021
- Invited talk: CCP-EM Spring Symposium, Oxfordshire, UK, April, 2021
- Invited talk: GlaxoSmithKline (GSK) Data Forum seminar series, London, UK, April, 2021
- Invited talk: Princeton University Applied Mathematics IDeAS Seminar, Princeton, NJ, Feb, 2021
- Invited talk: UIUC Coordinated Science Laboratory Student Conference (CSLSC), Champaign, IL, Feb, 2021
- Invited talk: Vienna BioCenter, Research Institute of Molecular Pathology (IMP) Seminar Series, Vienna, Austria, Nov, 2020
- (Cancelled) Invited talk: Machine Learning in Cryo-EM workshop, Institute of Mathematical Sciences, Singapore, Oct, 2020
- Invited talk: SciLifeLab Advanced Cryo-EM Seminar Series, Stockholm, Sweden, Sept, 2020
- Invited talk: Microscopy & Microanalysis, Milwaukee, WI, August, 2020
- (Cancelled) Invited talk: SIAM Conference on Imaging Science Cryo-EM Mini-symposium, Toronto, ON, July, 2020
- Invited talk: SBGrid Annual Symposium, Boston, MA, May, 2020
- (Cancelled) Invited talk: International Conference on Image Analysis in Three-dimensional Cryo-EM, Lake Tahoe, CA, March, 2020
- Invited talk: Relay therapeutics, Boston, MA, Feb, 2020
- Oral presentation (top 8% of submissions): Machine learning in Computational Biology (MLCB) meeting, Vancouver, BC, Dec 2019
- Poster: NeurIPS Learning Meaningful Representations of Life (LMRL) workshop, Vancouver, BC, Dec 2019
- Invited talk: Harvard Cryo-EM Club, Cambridge, MA, Dec 2019
- Poster: Janelia Women in Computational Biology Meeting, Ashburn, VA, Nov 2019
- Invited talk: New England CryoEM symposium, Worcester, MA, October 2019
- Poster: Flatiron Institute Computational Cryo-EM Workshop, New York, NY, August 2019
- Poster: MIT Biology Departmental Retreat, Cape Cod, MA, June 2019

Testing the limits of modern heterogeneous reconstruction algorithms: The autophagy initiation complex.

- Poster: Purdue Cryo-EM Symposium, Lafayette, IN, Nov 7, 2018

From silicon to medicine: Core challenges of using molecular dynamics for early-stage drug discovery.

- Talk: Out in STEM National Conference, Pittsburgh, PA, Nov.14, 2015.

Optimizing molecular visualization for drug discovery.

- Talk: Grace Hopper Annual Conference, Houston, TX, Oct. 14 2015

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

- Talk: AIChE Annual Meeting, San Francisco, CA, Nov. 6, 2013

ACADEMIC SERVICE

Reviewer

- Neural Information Processing Systems (NeurIPS)
- International Conference on Learning Representations (ICLR)
- Machine Learning in Computational Biology (MLCB)
- IEEE Transactions on Computational Biology and Bioinformatics
- IEEE Transactions on Computational Imaging
- Journal of Physical Chemistry Letters
- Scientific Reports

Meetings

- Co-organizer, Machine Learning in Structural Biology Workshop at NeurIPS 2021
- Co-organizer and program chair, Machine Learning in Structural Biology Workshop at NeurIPS 2020
- Co-organizer, MIT Biology career seminar series 2018-2019

Mentorship

- MIT iGEM synthetic biology team 2021
- Andy Tso, EECS MEng student 2020-2021
- Graduate student panelist, Computational and Systems Biology PhD Program 2019, 2020, 2021

TEACHING

- 7.57 Graduate Quantitative Biology TA with Prof. Joey Davis Spring, 2019
 ChE 2216 Modeling and Simulation TA with Prof. Michael Shirts Spring, 2013

GRANTS AND FELLOWSHIPS

- 2018 MIT J Clinic for Machine Learning and Health. *Deep Generative Models for Cryo-EM Reconstruction of Heterogeneous Biomolecular Structures* (to Prof. B. Berger and Prof. J. Davis)
 2017 NSF Graduate Research Fellowship Award
 2014 NSF Graduate Research Fellowship Award (Declined)

AWARDS

- 2019 Best paper award at Machine Learning in Computational Biology
 2019 Teaching Award from MIT Biology Department
 2019 Best poster award at MIT Biology Department Retreat
 2014 Louis T. Rader Chemical Engineering Prize: Awarded from UVA Dept. of ChemE
 2014 American Institute of Chemists Award: Awarded from UVA Dept. of ChemE
 2013 Barry M. Goldwater Scholarship
 2012, 2013 Astronaut Scholarship