

YILAI LI

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Education

Ph.D. in Biophysics University of Michigan Thesis: Super-resolution imaging of the DNA replisome in live <i>Bacillus subtilis</i> Advisor: Dr. Julie S. Biteen	ANN ARBOR, MI, USA 2013 – 2018
M.S. in Computer Science Georgia Institute of Technology	ONLINE 2020 – 2023
M.A. in Statistics University of Michigan	ANN ARBOR, MI, USA 2015 – 2018
B.S. in Biological Sciences Fudan University Thesis: Conformational dynamics of cryptochrome using single-molecule FRET Advisor: Dr. Yan-Wen Tan	SHANGHAI, CHINA 2009 – 2013

Research Experience

Research Scientist, ByteDance Seed, AI-for-Science 2023 – present

Pioneering AI-driven cryo-electron microscopy (cryo-EM) algorithms, from structure-constrained reconstruction to a flow-matching foundation model with real-data applications.

- *Group leader: Dr. Quanquan Gu*
 - Developed *cryoSTAR*, an algorithm for cryo-EM 3D reconstruction of datasets with continuous heterogeneity, by incorporating user-provided atomic models as structural priors within a variational autoencoder (VAE) framework.
 - Built *cryoFM*, the first foundation model for cryo-EM using flow matching, trained on high-quality density maps from the Electron Microscopy Data Bank (EMDB).
 - Applied *cryoFM* to experimental cryo-EM datasets, addressing practical challenges in the pipeline from 3D refinement to map modification and enabling controllable density refinement and enhancement.
 - Implemented a PyTorch-based framework for the expectation-maximization (EM) algorithm in single-particle cryo-EM, providing a modular and extensible platform for reconstruction and refinement.
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Willis Life Sciences Fellow, Life Sciences Institute, University of Michigan 2018 – 2023

Developed deep learning algorithms and workflows to help improve and automate cryo-electron microscopy (cryo-EM) data acquisition and processing.

- *Advisor: Dr. Michael A. Cianfrocco*
- Developed automatic pipelines with deep learning tools for cryo-EM data processing.

- Developed algorithms for automatic data acquisition with supervised classification/regression and deep reinforcement learning (*cryoRL*).
- Led a team of web developers to create a modern and flexible web-based user interface for cryo-EM software.

Ph.D in Biophysics, University of Michigan

2013 – 2018

Thesis: Super-resolution imaging of the DNA replisome in live *Bacillus subtilis*.

- Advisor: Dr. Julie S. Biteen
- Used super-resolution fluorescence microscopy (PALM) to quantify the behaviors of replisomal proteins in live *Bacillus subtilis* cells.
- Characterized the diffusive behaviors of different replisome proteins at the single-molecule level with quantitative models.
- Applied hierarchical Bayesian mixed Hidden Markov Models to single-molecule time series data to quantify the number of molecules in a cluster.

Undergraduate researcher, Department of Physics, Fudan University

2009 – 2013

Thesis: Conformational dynamics of cryptochrome using single-molecule FRET

- Advisor: Dr. Yan-Wen Tan

Undergraduate researcher, Stockholm University

2012

Studied the structural information of an ABC transporter protein.

- Advisor: Dr. Gunnar von Heijne

Publications

[†] indicates equal contribution.

Zhou, Y.[†], Li, Y.[†], Yuan, J.[†], & Q. Gu. CryoFM: A Flow-based Foundation Model for Cryo-EM Densities. In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2025. doi: <https://doi.org/10.48550/arXiv.2410.08631>

Li, Y.[†], Zhou, Y.[†], Yuan, J.[†], Ye, F., & Q. Gu. CryoSTAR: leveraging structural priors and constraints for cryo-EM heterogeneous reconstruction. *Nat Methods* (2024). doi: <https://doi.org/10.1038/s41592-024-02486-1>

Zhou, Y.[†], Li, Y.[†], Yuan, J.[†], Ye, F., & Q. Gu. CryoSTAR: Cryo-EM Heterogeneous Reconstruction of Atomic Models with Structural Regularization. In *NeurIPS 2023 Workshop on New Frontiers of AI for Drug Discovery and Development*.

Li, Y.[†], Fan, Q.[†], Xu, Z., Lee, E. R., Cohn, J., Demers, V., ... & Vos, S. M. (2023). Optimized path planning surpasses human efficiency in cryo-EM imaging. *eLife* 12:RP88640. doi: <https://doi.org/10.7554/eLife.88640.1>

Fan, Q.[†], Li, Y.[†], Yao, Y., Cohn, J., Liu, S., Xu, Z., ... & Cianfrocco, M. (2024). CryoRL: Reinforcement learning enables efficient cryo-em data collection. In *Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision* (pp. 7892-7902). doi: <https://doi.org/10.48550/arXiv.2204.07543>

- Xu, Z., Fan, Q., Li, Y., Lee, E. R., Cohn, J. M., Tewari, A., ... & Cianfrocco, M. Coupling Semi-supervised Learning with Reinforcement Learning for Better Decision Making—An application to Cryo-EM Data Collection. In *NeurIPS 2023 AI for Science Workshop*.
- Bepler, T., Borst, A. J., Bouvette, J., Cannone, G., Chen, S., Cheng, A., ... & Potter, C. S. (2022). Smart data collection for CryoEM. *Journal of Structural Biology*, 214(4), 107913. doi: <https://doi.org/10.1016/j.jsb.2022.107913>
- Li, Y., & Cianfrocco, M. A. (2022). Cloud computing platforms to support cryo-EM structure determination. *Trends in Biochemical Sciences*, 47(2), 103-105. doi: <https://doi.org/10.1016/j.tibs.2021.11.005>
- Li, Y., Cash, J. N., Tesmer, J. J., & Cianfrocco, M. A. (2020). High-throughput cryo-EM enabled by user-free preprocessing routines. *Structure*, 28(7), 858-869. (**Cover article**). doi: <https://doi.org/10.1016/j.str.2020.03.008>
- Cash, J. N., Kearns, S., Li, Y., & Cianfrocco, M. A. (2020). High-resolution cryo-EM using beam-image shift at 200 keV. *IUCr*, 7(6), 1179-1187. doi: <https://doi.org/10.1107/s2052252520013482>
- Li, Y., Chen, Z., Matthews, L. A., Simmons, L. A., & Biteen, J. S. (2019). Dynamic exchange of two essential DNA polymerases during replication and after fork arrest. *Biophysical journal*, 116(4), 684-693. (**Cover article**). doi: <https://doi.org/10.1016/j.bpj.2019.01.008>
- Isaacoff, B. P., Li, Y., Lee, S. A., & Biteen, J. S. (2019). SMALL-LABS: Measuring single-molecule intensity and position in obscuring backgrounds. *Biophysical Journal*, 116(6), 975-982. doi: <https://doi.org/10.1016/j.bpj.2019.02.006>
- Li, Y., Schroeder, J. W., Simmons, L. A., & Biteen, J. S. (2018). Visualizing bacterial DNA replication and repair with molecular resolution. *Current opinion in microbiology*, 43, 38-45. doi: <https://doi.org/10.1016/j.mib.2017.11.009>
- Liao, Y., Li, Y., Schroeder, J. W., Simmons, L. A., & Biteen, J. S. (2016). Single-molecule DNA polymerase dynamics at a bacterial replisome in live cells. *Biophysical journal*, 111(12), 2562-2569. doi: <https://doi.org/10.1016/j.bpj.2016.11.006>

Selected Honors and Awards

Willis Life Sciences Fellow	2019–2022
Rackhan Travel Grant	2016, 2015 & 2014
Biophysical Society Travel Award	2015
Rackham Graduate Student Research Grant	2014

Conferences and Presentations

American Crystallographic Association	Invited oral presentation, 2024
Neural Information Processing Systems workshop (AI4D3)	Poster presentation, 2023
Machine Learning in cryo-EM	Invited oral presentation, 2022
American Crystallographic Association	Two oral presentations, 2022
8th Semi-Annual New England CryoEM Symposium	Oral presentation, 2022
Workshop on Smart Data Collection for CryoEM	Invited oral presentation, 2022

4th International Symposium on Cryo-3D Image Analysis	<i>Poster presentation, 2022</i>
M&M Microscopy & MicroAnalysis	<i>Poster presentation, 2020</i>
2019 Cryo-EM Symposium	<i>Poster presentation, 2019</i>
NYC Computational Cryo-EM Summer Workshop	<i>Poster presentation, 2019</i>
M&M Microscopy & MicroAnalysis	<i>Poster presentation, 2019</i>
Bio-IT World Conference & Expo	2019
Biophysical Society Annual Meeting	<i>Poster presentation, 2018</i>
Biophysical Society Annual Meeting	<i>Poster presentation, 2017</i>
Biophysical Society Annual Meeting	<i>Poster presentation, 2016</i>

Teaching Experience

Graduate Student Instructor (GSI) for five semesters at the University of Michigan.	2014 – 2017
• General Chemistry • General Chemistry Lab • Physical Chemistry • Organic Chemistry Lab II	

Leadership and Mentoring

- Led a team of 11 web developers on the *cryoHub* project, overseeing UI development for cryo-EM software, with responsibilities in project management, budgeting, and recruitment.
- Mentored four undergraduate and graduate students in the Biteen and Cianfrocco labs, providing guidance on research and professional development.
- Supervised three interns at ByteDance Seed, supporting their technical growth and project contributions.