Xiaochen Du

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EDUCATION

Massachusetts Institute of Technology (MIT) Cambridge, MA
PhD Chemical Engineering, Computational Science and Engineering Sep 2021 - Aug 2026 (expected)
National Science Foundation (NSF) Graduate Research Fellow
Advisors: Rafael Gómez-Bombarelli, Martin Z. Bazant
Thesis: Accelerating thermodynamic sampling of material surfaces and interfaces

Duke University Durham, NC
BS Computer Science, AB Chemistry, *summa cum laude* Aug 2017 - Dec 2020
Duke Faculty Scholar (highest undergraduate honor)
Alex Vasilos Memorial Award (for excellence in computer science research)

RESEARCH EXPERIENCE

MIT, Department of Materials Science and Engineering Cambridge, MA
Graduate Researcher, Rafael Gómez-Bombarelli Group Jan 2022 - present
- Developing deep learning-based methods in PyTorch to accelerate atomistic simulations and materials discovery in fields such as catalysis, batteries, and other sustainability applications
- Scaling and optimizing graph neural network-based force fields and Transformer-based generative models to study surface reconstructions, enhancing model efficiency and accuracy
- Curating surface reconstruction datasets through high-throughput thermodynamics sampling and large-scale DFT calculations for community use
- Open-sourced new Python packages and expanded existing repositories by more than 10k lines (https://github.com/learningmatter-mit)

Duke University, Department of Computer Science Durham, NC
Researcher and Software Engineer, Alberto Bartesaghi Group Jan 2020 - Apr 2021
- Optimized protein cryo-EM image reconstruction pipeline by integrating denoising algorithms, deep learning models, and statistical inference methods
- Engaged experimental biochemists and software engineers to redesign computational workflow
- Scaled analysis workflows to handle terabytes of noisy image data across 100+ compute nodes
- Led a team of 5 to refactor 30k lines of code and open-source Python codebase (https://github.com/nextpyp)

Duke University, Department of Mechanical Engineering and Materials Science Durham, NC
Undergraduate Researcher and Software Engineer, Volker Blum Group Sep 2017 - Dec 2019
- Developed and open-sourced a curated materials database (https://github.com/HybriD3-database/MatD3) using Python and Django, improving verifiability and reproducibility (https://materials.hybrid3.duke.edu)
- Processed and analyzed high-dimensional data from both experimental and computational sources, including adsorption spectra, X-ray diffraction data, and band structures
- Directed a cross-functional team of 15+ researchers across three institutions and five departments

INDUSTRY EXPERIENCE

Apple Cupertino, CA
Incoming Battery Analytics and ML Intern May - Aug 2025
- Research deep learning and generative models to optimize battery performance
- Develop machine-learning accelerated atomistic simulations to improve battery design

Emerald Cloud Lab South San Francisco, CA
Scientific Computing Intern May - Aug 2019
- Upgraded data and image analysis methods in Wolfram language to handle more experiment types, enhancing the automation of scientific wet-lab experiments

SELECTED JOURNAL & WORKSHOP PUBLICATIONS

[J1] **Du, X.**, Liu, M., Peng, J., Chun, H., Hoffman, A., Yildiz, B., Li, L., Bazant, M.Z. & Gómez-Bombarelli, R. (2025). Accelerating and enhancing thermodynamic simulations of electrochemical interfaces.
Preprint: https://arxiv.org/abs/2503.17870.

[W1] **Du, X.**, Liu, S. & Gómez-Bombarelli, R. (2024). Scaling autoregressive models for lattice thermodynamics. *NeurIPS 2024 AI for Accelerated Materials Design Workshop*. https://openreview.net/forum?id=JynhVjza4n

[J2] **Du, X.**, Damewood, J.K., Lunger, J.R., Millan, R., Yildiz, B., Li, L. & Gómez-Bombarelli, R. (2023). Machine-learning-accelerated simulations to enable automatic surface reconstruction. *Nature Computational Science*, 3, 1044. DOI: 10.1038/s43588-023-00571-7
MIT News Feature: https://news.mit.edu/2023/mit-engineers-how-surfaces-materials-behave-1207

[J3] Liu, HF.*, Zhou, Y.*, Huang, Q., Piland, J., Jin, W., Mandel, J., **Du, X.**, Martin, J. & Bartesaghi, A. (2023). nextPYP: a comprehensive and scalable platform for characterizing protein variability in situ using single-particle cryo-electron tomography. *Nature Methods*, 20, 1909. DOI: 10.1038/s41592-023-02045-0 * equal contribution

[J4] Bouvette, J.*, Liu, HF.*, **Du, X.**, Zhou, Y., Sikkema, A.P., Mello, J.F.R., Klemm, B.P., Huang, R., Schaaper, R.M., Borgnia, M.J. & Bartesaghi, A. (2021). Beam image-shift accelerated data acquisition for near-atomic resolution single-particle cryo-electron tomography. *Nature Communications*, 12, 1957. DOI: 10.1038/s41467-021-22251-8 * equal contribution

[J5] Teo, R., **Du, X.**, Vera, H., Migliore, A. & Beratan, D. (2021). Correlation Between Charge Transport and Base Excision Repair in the MutY DNA Glycosylase. *J. Phys. Chem. B*, 125(1), 17. DOI: 10.1021/acs.jpcb.0c08598

[J6] Laasner, R., **Du, X.**, Tanikanti, A., Clayton, C., Govoni, M., Galli, G., Ropo, M. & Blum, V. (2020). MatD^3: A Database and Online Presentation Package for Research Data Supporting Materials Discovery, Design, and Dissemination. *Journal of Open Source Software*, 5(45), 1945. DOI: 10.21105/joss.01945

SELECTED PRESENTATIONS

[P1] **Accelerating thermodynamic simulations of electrochemical interfaces**
- Oral: American Chemical Society (ACS) Spring Meeting, San Diego, CA, US, Mar 2025
- Oral: Materials Research Society (MRS) Fall Meeting, Boston, MA, US, Dec 2024

[P2] **Scaling autoregressive models for lattice thermodynamics**
- Poster: AI4X Conference, Singapore, Jul 2025
- Poster: NeurIPS AI for Accelerated Materials Design (AI4Mat) Workshop, Vancouver, BC, Canada, Dec 2024

[P3] **Machine-learning accelerated simulations for heuristic-free surface reconstruction**
- Poster: JUAMI 2023: Materials for a Sustainable Future, Nairobi, Kenya, June 2023
- Oral: IPAM New Mathematics for the Exascale: Applications to Materials Science, Los Angeles, CA, US, May 2023 (delivered virtually)
- Oral: MRS Fall Meeting, Boston, MA, US, Nov-Dec 2022

HONORS & FELLOWSHIPS

Young National University of Singapore (NUS) Fellow (travel grant) (2024-2025); NSF Graduate Research Fellowship (2022-2025); Alex Vasilos Memorial Award (computer science research excellence, 2021); Phi Beta Kappa (2021); Duke Faculty Scholar (highest undergraduate honor, 2020)

TEACHING EXPERIENCE

10.426/626 Electrochemical Energy Systems TA, MIT (Spring 2024); CHEM 544 Statistical Mechanics TA, Duke (Fall 2020); ECE/CS 250 Computer Architecture TA, Duke (Fall 2018)

SKILLS

Research: Machine Learning, Computational Materials Science, Generative Modeling, Atomistic Simulations, Density-Functional Theory (DFT), High-Throughput Simulations
Coding: Python (PyTorch, Django, proficient), C++ (prior experience), Wolfram Language (prior experience)
Language: English, Mandarin Chinese

ACTIVITIES

Sidney-Pacific Graduate Residence Environment Chair (2023-2025); MIT Graduate Student Council Sustainability Subcommittee Co-chair (2022-2023)