

Xiaochen Du

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EDUCATION

Massachusetts Institute of Technology

Ph.D. Student, Computational Science and Engineering (Chemical Engineering)

Cambridge, MA
Sep 2021 - present

Duke University

B.S. Computer Science, A.B. Chemistry, *summa cum laude*

Durham, NC
Aug 2017 - Dec 2020

HONORS & FELLOWSHIPS

NSF Graduate Research Fellowship	2021
Alex Vasilos Memorial Award (for excellence in computer science research)	2021
Phi Beta Kappa	2021
Duke Faculty Scholar (highest undergraduate honor awarded by faculty)	2020

RESEARCH EXPERIENCE

Duke University, Department of Computer Science

Research Associate/Software Engineer, Alberto Bartesaghi Group

Durham, NC
Feb 2021 - Apr 2021

- Revamped in-house cryo-EM image analysis library, refactoring 30k lines of Python code
- Performed modularization, documentation, and containerization
- Implemented test-driven development, and a continuous integration (CI) pipeline

Duke University, Department of Computer Science

Researcher, Alberto Bartesaghi Group

Durham, NC
Jan 2020 - Dec 2020

- Improved cryo-EM image reconstruction using denoising, super resolution, and statistical inference
- Implemented new features into in-house Python package and made a mod of the *cisTEM* package

Duke University, Department of Mechanical Engineering and Materials Science

Researcher/Full-stack Software Engineer, Volker Blum Group

Durham, NC
Sep 2017 - Dec 2019

- Created a perovskite materials database with a Python Django web interface, leading to \$100,000 supplementary funding from NSF
- Managed the database effort by leading a team of 10+ students and postdocs across three institutions to expand the database to more than 500 entries
- Worked with another lab member to spin off the database into a general software stack

Duke University, Department of Chemistry

Researcher, David Beratan Group

Durham, NC
Jan - Jul 2020

- Analyzed the impact of mutations on protein electron transfer rates
- Improved an in-house Python package to allow parallel analysis of electron trajectories

Yale University, Department of Chemistry

Summer Researcher, Victor Batista Group

New Haven, CT
May - Aug 2018

- Explored machine learning (CNN, RNN) using Python Keras to predict quantum dynamics

INDUSTRY EXPERIENCE

Emerald Cloud Lab

Scientific Computing Intern

South San Francisco, CA
May - Aug 2019

- Worked at a series A startup with 50M capital automating chemistry and biology experiments, and moving them onto the cloud

- Added new data & image analysis functions in Wolfram language/Mathematica, and delivered software

TEACHING EXPERIENCE

CHEM 544 Statistical Mechanics TA for Prof. Patrick Charbonneau, Duke University	Fall 2020
ECE/CS 250 Computer Architecture TA for Prof. Benjamin Lee, Duke University	Fall 2018

SELECTED PUBLICATIONS

Bouvette, J.*, Liu, H.*, **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. *Nat. Commun.*, 12, 1957. * denotes equal contribution

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), 12.

Laasner, R., **Du, X.**, Tanikanti, A., Clayton, C., Govoni, M., Galli, G., Ropo, M. & Blum, V. (2020). MatD³: A Database and Online Presentation Package for Research Data Supporting Materials Discovery, Design, and Dissemination. *Journal of Open Source Software*, 5(45), 1945.

SELECTED PRESENTATIONS

HybriD³ and MatD³: Curated Materials Data for Hybrid Organic-Inorganic Perovskites and a General Software Stack for Materials Data

- Poster: Materials Research Society Spring & Fall Meeting, Remote, Nov 2020
- Poster: American Chemical Society National Meeting, Philadelphia, PA, Mar 2020 (Cancelled due to COVID-19)

Multi-frame Super-resolution Cryogenic-Electron Microscopy (Cryo-EM)

- Oral: Duke University Plus Programs Summer Expo, Remote, July 2020