Xiaochen Du

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EDUCATION

Massachusetts Institute of Technology — Cambridge, MA
Ph.D. Chemical Engineering, Computational Science and Engineering — Sep 2021 - present
Advisors: Rafael Gómez-Bombarelli, Martin Bazant

Duke University — Durham, NC
B.S. Computer Science, A.B. Chemistry, *summa cum laude* — 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

MIT, Department of Materials Science and Engineering — Cambridge, MA
Graduate Researcher, Rafael Gómez-Bombarelli Group — Jan 2022 - present

- Applying machine learning force fields to accelerate materials modelling
- Studying surface reconstruction of metal oxides for applications to catalysis and electrochemistry

Duke University, Department of Computer Science — Durham, NC
Research Associate/Software Engineer, Alberto Bartesaghi Group — 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 — Durham, NC
Undergraduate Researcher, Alberto Bartesaghi Group — 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 *cis*TEM package

Duke University, Department of Mechanical Engineering and Materials Science — Durham, NC
Undergraduate Researcher/Full-stack Software Engineer, Volker Blum Group — 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 — Durham, NC
Undergraduate Researcher, David Beratan Group — 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 — New Haven, CT
Summer Researcher, Victor Batista Group — May - Aug 2018

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

INDUSTRY EXPERIENCE

Emerald Cloud Lab South San Francisco, CA
Scientific Computing Intern 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

Du, X., Damewood, J.K., Lunger, J.R., Millan, R., Yildiz, B., Li, L., & Gómez-Bombarelli, R. (2023). Machine-learning-accelerated simulations enable heuristic-free surface reconstruction. arXiv:2305.07251

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), 17.

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.

SELECTED PRESENTATIONS

Machine-learning-accelerated simulations for heuristic-free surface reconstruction

- Oral: IPAM New Mathematics for the Exascale: Applications to Materials Science, Los Angeles, CA, May 2023

Sampling the Thermodynamics of Material Surfaces with Markov chain Monte Carlo and Machine Learning Potential

- Oral: Materials Research Society Fall Meeting, Boston, MA, Nov-Dec 2022
- Poster: MIT Lincoln Laboratory GraphEx Symposium, Remote, May 2022

HybriD^3 and MatD^3: 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

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

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