Austin H. Cheng

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EDUCATION

University of Toronto **Toronto, Ontario**
PhD Student in Chemistry Sep 2021-Present
Supervisor: Alán Aspuru-Guzik

University of Virginia **Charlottesville, Virginia**
B.S. in Chemistry with Specialization in Chemical Physics Aug 2017-May 2021
with High Distinction GPA: 3.93/4.00
B.A. in Computer Science

RESEARCH EXPERIENCE

Group SELFIES: A Robust Fragment-based Molecular String Representation **2022**
Supervisors: Santiago Miret, Alán Aspuru-Guzik University of Toronto

- Implemented a version of SELFIES that adds tokens that represent functional groups or entire substructures while maintaining robustness
- Improves compactness, interpretability, and molecular generation
- Mentored undergraduate student Andy Cai

Spectral Tensor Field Networks **2022**
Professor: Roger Grosse Course project for Neural Network Training Dynamics

- Incorporated SE(3)-equivariance into spectral learning to simultaneously find the ordered eigenstates of molecules, while improving convergence

Dynamic self-assembly of a colloidomer under a time-oscillating potential **2020-2021**
Supervisor: Kateri DuBay University of Virginia, Distinguished Majors Thesis

- Programmed and analyzed Brownian dynamics simulations of a colloidomer with acidic and basic monomers under time-oscillating pH, which self-assembles into non-equilibrium dissipative structures
- Found that structures which appear frustrated in the effective time-averaged landscape can be annealed by a medium-fast oscillation period, even though these are all dissipative structures

PUBLICATIONS & POSTERS

Cheng, A. H.*, Cai, A.*, Miret, S., Malkomes, G., Phielipp, M., & Aspuru-Guzik, A. (2022) Group SELFIES: A Robust Fragment-Based Molecular String Representation. Digital Discovery. (Accepted at NeurIPS 2022 AI4Mat Workshop)

Mayer, K. J., Pate, B., Patrinely, E., Pert, E., **Cheng, A.**, Baugh, K., ... & Simon, I. (2019, June). The Feasibility of Determining the Carbon Framework Geometry of a Molecule from Analysis of the CARBON-13 Isotopologue Rotational Spectra in Natural Abundance. In *74th International Symposium on Molecular Spectroscopy* (Poster)

Cheng, A. H., Kim, C. J., Wang, A. Y., Zhu, X., Jia, Q., & DuBay, K. H. (2019). Simulating the Folding States of Lattice Proteins within an Oscillatory Environment. *Biophysical Journal*, *116*(3), 476a. (Poster)

AWARDS & ACHIEVEMENTS

ACS Undergraduate Award in Physical Chemistry 2021
Pinnacle Hackathon, the Olympics of Hackathons, Participant 2021
RapBox: an AI-powered tool to generate an entire rap music video from just a title
HooHacks 2021, Overall Winner 2021
RealTalk: a web app that uses deep learning to let users have a conversation with historical figures
Accepted to NYU-MRSEC Summer REU (cancelled due to COVID-19) 2020
Lawrence Harrison Kilmon and May Lewis Kilmon Dean's Scholarship 2020
Claiborne and Martha Whitworth Scholarship Dean's Scholarship 2019
Randolph Preston Pillow Fund for Excellence Dean's Scholarship 2018
Eagle Scout 2017
Service Project: Organized construction of an outdoor high school classroom amphitheatre
UVa College of Arts & Sciences Echols Scholar 2017
National Chemistry Olympiad Exam Qualified Student (1 of 18 in DC area) 2017
Virginia's Governor's School for Agriculture 2016

TEACHING

University of Toronto, Teaching Assistant
Chemistry: Physical Principles - Lab Demonstrator Jan 2023-Apr 2023
Introduction to the Theory of Computation Sep 2022-Dec 2022
Chemistry: Physical Principles Sep 2022-Dec 2022
Introduction to Computer Science - Lab Demonstrator Jan 2022-Apr 2022
Chemistry: Physical Principles - Lab Demonstrator Sep 2021-Dec 2021

University of Virginia, Teaching Assistant
Introduction to Algorithms Jan 2021-May 2021
Introduction to Physical Chemistry I: Quantum Mechanics Aug 2019-Dec 2019

SKILLS

Proficient: Python, NumPy, PyTorch, JAX, Streamlit, Git, Unix/Linux, LaTeX
Familiar: JavaScript, Haskell, C++
Relevant Coursework: Automated Reasoning with Machine Learning, Neural Network Training Dynamics, Machine Learning for Vision and Language, Statistical Learning and Graphical Models