

Chu Xin (Cloris) Cheng

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EDUCATION

Stanford University

Ph.D. Computer Science

Stanford, CA

Sep. 2026 – Present

California Institute of Technology

B.S. Computer Science

Pasadena, CA

Sep. 2021 – Jun. 2025

- **Cumulative GPA:** 4.3

LIST OF PUBLICATIONS

Atomic Diffusion Models for Small Molecule Structure Elucidation from NMR Spectra

Ziyu Xiong, Yichi Zhang, Foyez Alaaddin, Chu Xin Cheng, Joon Soo An, Mohammad R. Seyedsayamdost, Ellen D. Zhong

Neural Information Processing Systems (NeurIPS), 2025.

Available: <https://openreview.net/pdf?id=STsjfx2cee>

How to Unlock Time Series Editing? Diffusion-Driven Approach with Multi-Grained Control

Hao Yu*, Chu Xin Cheng*, Runlong Yu, Yuyang Ye, Shiwei Tong, Zhaofeng Liu, Defu Lian

arXiv preprint, 2025.

Available: <https://arxiv.org/pdf/2506.05276>

Preferential Bayesian Optimization with Multiple Mixed Objectives

Raul Astudillo, Kejun Li, Maegan Tucker, Chu Xin Cheng, Aaron Ames, Yisong Yue

Transactions on Machine Learning Research (TMLR), 2025.

Available: <https://openreview.net/pdf?id=mjsoESaWDH>

Practical Bayesian Algorithm Execution via Posterior Sampling

Chu Xin Cheng*, Raul Astudillo*, Thomas Desautels, Yisong Yue

Neural Information Processing Systems (NeurIPS), 2024.

Available: <https://arxiv.org/pdf/2410.20596>

Improving sample efficiency of high dimensional Bayesian optimization with MCMC

Zeji Yi*, Yunyue Wei*, Chu Xin Cheng*, Kaibo He, Yanan Sui

Learning for Dynamics & Control Conference (L4DC), 2024.

Available: <https://proceedings.mlr.press/v242/yi24a/yi24a.pdf>

HONORS AND AWARDS

Hertz Fellow

2025

Fannie and John Hertz Foundation

- Awarded annually to the nation's most promising graduate students in the applied sciences, mathematics, and engineering; provides five years of funding.

Bhansali Family Prize in Computer Science

2025

California Institute of Technology

- Awarded to an undergraduate for outstanding research in computer science, selected by a faculty committee.

Finalist, Undergraduate Operations Research Prize

2024

Institute for Operations Research and the Management Sciences

- Honors original undergraduate research in operations research or management science; finalists present at the INFORMS Annual Meeting.

Jack E. Froehlich Memorial Award

2024

California Institute of Technology

- Awarded to a junior in the top 5% of their class who shows outstanding promise for a creative professional career.

Henry Ford II Scholar Award

2024

California Institute of Technology

- Awarded to engineering students with the best academic record after three years of study.

WORK AND RESEARCH EXPERIENCES

Quantitative Researcher, Seven Research

Jul. 2025 – Aug. 2026

Shanghai, China / New York, NY

- Developed machine learning models for stock return prediction.

Machine Learning Researcher, Gridmatic

Spring 2025

Cupertino, CA

- Research on generative modeling for time series forecasts; enhanced day-ahead electricity-price forecasting by incorporating super-resolution features. Curated datasets and built models for predicting power grid congestion.

Machine Learning Researcher, Yisong Yue's Group

2022 - 2024

California Institute of Technology / Lawrence Livermore National Lab

- Project 1, 2022** Generalized Bayesian optimization to learn from preference feedback under the dueling bandits framework, including continuous spaces via Gaussian processes. Developed an algorithm using Langevin dynamics and Kalman filtering on the posterior to leverage gradient feedback.
- Project 2, 2023** Contributed to the first theoretical framework for multi-attribute preferential Bayesian optimization, applied to exoskeleton gait optimization. Designed an algorithm using Chebyshev scalarization to produce Pareto-optimal actions.
- Project 3, 2023** Investigated machine learning methods for antibody design. Applied feature conformal prediction to graph neural networks to obtain confidence intervals with guaranteed coverage for fitness modeling.
- Project 4, 2024** Developed PSBAX, a posterior-sampling algorithm for inferring properties of unknown functions. Demonstrated superior performance across multiple domains, including real-world protein engineering datasets, and contributed to its convergence analysis. Collaborated with Lawrence Livermore National Lab to apply PSBAX to antibody portfolio optimization.

Machine Learning Researcher, Zhong Lab

2024

Princeton University

Summer Undergraduate Research Fellowship

- Research with Prof. Ellen Zhong on predicting small molecule structures from NMR spectra to accelerate natural product discovery. Achieved 98.9% accuracy using a multilabel classifier to identify amino acid groups in peptides from synthetic NMR spectra.

Machine Learning Researcher, Rigorous Systems Research Group

2022 - 2023

California Institute of Technology

- Research with Prof. Adam Wierman on online policy selection in optimization and control. Investigated generalizing optimization algorithms to nonlinear dynamical systems with non-convex reward functions.

Research Assistant

2022

California Institute of Technology / Tsinghua University

Summer Undergraduate Research Fellowship

- Research with Prof. Yanan Sui on high-dimensional Bayesian optimization with Gaussian processes, applied to spinal stimulation. Used Markov chain Monte Carlo and Langevin dynamics to sample from intractable posteriors, and devised an algorithm that maintains an adaptive mesh over a high-dimensional action space.

Intern, Tencent (Tencent Xinghuo Program)

2021 - 2022

Shenzhen, Tencent Quantum Lab

- Reproduced the quantum approximate optimization algorithm using TensorFlow and Qiskit; studied quantum algorithms including Grover search and variational methods.

TEACHING EXPERIENCES

Teaching Assistant

2023 - 2024

California Institute of Technology

- Led recitations, held weekly office hours, and wrote and graded problem sets for classes of about 100 students.
- Courses: Data Mining and Machine Learning (Winter 2023, 2024), Statistical Inference (Spring 2023, 2024), Introduction to Probability Models (Fall 2023), Applied Linear Algebra (Fall 2024).

TECHNICAL SKILLS

Languages: Python, C, Java, OCaml, Swift, MATLAB.

ML Packages: PyTorch, TensorFlow, Pandas, SciPy.