Cher-Tian Ser

chertianser.github.io
ctser@cs.toronto.edu
Google Scholar
LinkedIn
GitHub

Profile

PhD student working at the intersection of computational chemistry and machine learning for the discovery of catalytic and energy materials. Dedicated to understanding nature better via data-driven approaches. Skilled user of quantum chemistry software and at developing scripted workflows for dataset generation. Passionate about science communication and mentorship.

Skills and Proficiencies

Quantum Chemistry

- Extensive experience in semiempirical methods, density functional theory, transition state theory and cutting-edge multireference methods for computing molecular and material properties.
- Published first-author papers on catalytic mechanisms, quantitative structure-activity relationships and high-throughput computational materials screening.
- Expertise in Gaussian, ORCA, OpenMolcas and VASP quantum chemical software suites.

Machine Learning & Programming

- Deployed quantum chemical variables and molecular representations as input for various supervised learning approaches to accurately predict chemical properties.
- Model selection and validation for test-set generalization on non-random dataset splittings.
- Adept at visualizing high-dimensional datasets with t-SNE, UMAP and graph networks.

Workflows

- Automated high-throughput property calculations for 100,000s of molecules and materials, and complicated mechanistic analysis of metal-catalyzed chemical reactions.
- Structural manipulation, input generation, error handling and data processing using Python, Bash and open-source packages.
- Experienced in high-performance parallel computing and library compilation on compute clusters with SLURM and PBS job schedulers.

Leadership & Mentorship

- Developed and executed lesson plans for underprivileged and remote Indigenous communities in Ontario (with Pueblo Science).
- Coordinated teaching efforts as Head TA across 30 TAs, and awarded for teaching excellence.
- Chair of Machine Learning subgroup meetings.
- Elected House Captain of USP, and Vice-Captain of USP Tchoukball.

Education

Doctor of Philosophy (in progress) 2020 - present
University of Toronto, Canada
Physical Chemistry

- Supervised by Prof. Alán Aspuru-Guzik

Bachelor of Science Sep 2015 - May 2019
National University of Singapore, Singapore
Chemistry (Materials Chemistry Specialization)

- Highest Distinction (GPA 4.77/5.00)
- University Scholars Programme (USP), a selective Honors College program

Work Experience

Machine Learning Intern May 2025 - Aug 2025
Osmo, New York, USA

- Machine learning for olfactory properties of molecules and mixtures

Research Engineer Sep 2019 - Aug 2020
IHPC, A*STAR, Singapore

- High-throughput computations for the discovery of high-temperature piezoelectric materials

Selected Publications

1. **Ser, C. T.***, Hao, H.*; Pablo-García, S.; Jorner, K.; Li, S.; Pollice, R.; Aspuru-Guzik, A., Bulky ligands promote palladium-catalyzed protodeboronation. *J. Am. Chem. Soc.*, **2025**, *147* (47), 43884–43901
2. Wang, H.*; Skreta, M.*; **Ser, C. T.**; …, Du, Y.; Aspuru-Guzik, A.; Neklyudov, K.; ; Zhang, C., Efficient Evolutionary Search Over Chemical Space with Large Language Models. *ICLR*, **2025**
3. Tom, G.*; **Ser, C. T.***; Rajaonson, E. M.*; Lo, S.; Park, H. S.; Lee, B. K.; Sanchez-Lengeling, B., Does This Smell The Same? Learning Representations of Olfactory Mixtures Using Inductive Biases. *Mach. Learn.: Sci. Technol.*, **2025**
4. Zou, Y., Cheng, A. H., Aldossary, A., …, **Ser, C. T.**, …, Bernales, V., Aspuru-Guzik, A., El Agente: An autonomous agent for quantum chemistry. *Matter* **2025**, *8* (7), 102263.
5. Strieth-Kalthoff, F.*; Hao, H.*; …, **Ser, C. T.**; …, Adachi, C.; Grzybowski, B. A.; Cronin, L.; Hein, J. E.; Burke, M. D.; Aspuru-Guzik, A., Delocalized, Asynchronous, Closed-Loop Discovery of Organic Laser Emitters. *Science*, **2024**, *384* (6697), eadk9227.
6. Pires-Valverde, D.*; **Ser, C. T.***, Ricci, G.; Jorner, K.; Pollice, R.; Aspuru-Guzik, A.; Olivier, Y. Computational Investigations of the Detailed Mechanism of Reverse Intersystem Crossing in Inverted Singlet-Triplet Gap Molecules. *ACS Appl. Mater. Interfaces*, **2024**, *16* (49), 66991–67001
7. Pollice, R.; dos Passos Gomes, G.; Aldeghi, M.; Hickman, R. J.; Krenn, M.; Lavigne, C.; Lindner-D'Addario, M.; Nigam, A.; **Ser, C. T.**; Yao, Z.; Aspuru-Guzik, A., Data-Driven Strategies for Accelerated Materials Design. *Acc. Chem. Res.* **2021**, *54* (4), 849-860.
8. **Ser, C. T.**; Yang, H.; Wong, M. W., Iodoimidazolinium-Catalyzed Reduction of Quinoline by Hantzsch Ester: Halogen Bond or Brønsted Acid Catalysis, *J. Org. Chem.*, **2019**, *84*, 10338.

Patents

1. Aguilar-Granda, A.; Batey, R. A.; …; **Ser, C. T.**; …; Aspuru-Guzik, A. Cationic viologen derivatives and use thereof in redox flow batteries. (patent pending)

Selected Conferences

- **Apr 2025, ICLR, Singapore**
  - Efficient evolutionary search over chemical space with large language models (Poster)
  - Learning representations of olfactory mixtures using inductive biases. (Oral, AI4Mat)
- **Aug 2024, ACS Fall, Denver, Colorado, USA**
  - Bulky ligands promote palladium-catalyzed protodeboronation (Oral)

Open-Source Software

- **deepchem**, an open-source Python package for deep learning in chemistry (Contributor)
  - Molecular fingerprint splitting for machine learning models
- **crest**: molecular conformer generation via metadynamics (Contributor)

Teaching Experience

- **CHM135**, Chemistry: Physical Principles
  - Head TA, Tutor and Computational Lab TA
- **CHM136**, Introductory Organic Chemistry I
- **CHM247**, Introductory Organic Chemistry II

Selected Awards

- **Jun-2025 & Jul-2023**, Chemistry Teaching Excellence Award, UofT
- **Apr-2025**, GSEF ChemClub Graduate Scholarship, UofT
- **May-2024**, ChemClub Chemistry Education Award, UofT