


CHER-TIAN SER

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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

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

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

Research Assistant May 2019 - Aug 2019
National University of Singapore, Singapore

- Investigation of intramolecular halogen bonding on thermally-activated delayed fluorescence

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