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 molecular 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.
- Coordinated teaching efforts as Head TA.
- 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.**; Tan, T. L, Uncovering compounds with promising piezoresistive properties via high-throughput first-principles survey. *Materials Today Communications* **2023**, *34*, 105240.
2. Cao, Y; **Ser, C. T.;** Skreta, M.; Jorner, K.; Kusanda, N.; Aspuru-Guzik, A., Reinforcement learning supercharges redox flow batteries. *Nature Machine Intelligence* **2022**, *4* (8), 667-668. (News & Views)
3. Seifrid, M.; Pollice, R.; Aguilar-Granda, A.; Chan, Z. M.; Hotta, K.; **Ser, C. T.**; Vestfrid, J.; Wu, T. C.; Aspuru-Guzik, A., Autonomous Chemical Experiments: Challenges and Perspectives on Establishing a Self-Driving Lab. *Accounts of Chemical Research* **2022**, *55* (17), 2454-2466.
4. 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. *Accounts of Chemical Research* **2021**, *54* (4), 849-860.
5. **Ser, C. T.**; Mak, A. M., Wejrzanowski, T., Tan, T. L., Designing Piezoresistive Materials from First-Principles: Dopant Effects on 3C-SiC, *Computational Materials Science* **2021**, *186*, 110040
6. **Ser, C. T.**; Žuvela, P.; Wong, M. W., Prediction of Corrosion Inhibition Efficiency of Pyridines and Quinolines on an Iron Surface using Machine Learning-Powered Quantitative Structure-Property Relationships, *Applied Surface Science*, **2020**, *512*, 145612
7. **Ser, C. T.**; Yang, H.; Wong, M. W., Iodoimidazolinium-Catalyzed Reduction of Quinoline by Hantzsch Ester: Halogen Bond or Brønsted Acid Catalysis, *The Journal of Organic Chemistry*, **2019**, *84*, 10338.

Conferences

- **Aug 2022, Accelerate Conference, Toronto, Ontario, Canada**
  - Palladium-catalyzed Protodeboronation of Boronic Acid Derivatives (Poster)
- **May 2019, 2nd Chemistry National Meeting, Singapore**
  - Machine Learning the Corrosion Inhibition Efficiency of Organic Compounds (Poster)

Selected Awards

- **07-2023**, Chemistry Teaching Excellence Award, UofT
- **08-2019**, National Science Scholarship (PhD), A*STAR (declined)
- **07-2019**, Lijen Industrial Development Medal, NUS
- **05-2019**, USP President's Honour Roll, NUS
- **05-2019**, USP Best Performing Student in Sciences and Technology Domain, NUS
- **05-2019**, Science Dean's List, NUS
- **05-2018**, Science Dean's List, NUS
- **01-2018**, A*STAR Undergraduate Scholarship
- **09-2017**, USP Senior Honour Roll, NUS

Open-Source Software

- **deepchem**, an open-source Python package for deep learning in chemistry (Contributor)
  - Implemented fixes to k-fold molecular fingerprint splitting
- **cheapocrest**: quick molecular conformer generation based on `openbabel` and `xtb`.
  - In development

Languages

Native	**Working Proficiency**	**Elementary**
English	Mandarin Chinese	Korean, French

Teaching Experience

- **CHM135**, Physical Chemistry for Life Sciences
  - Head TA, Tutor and Computational Lab TA (4 sessions)
- **CHM136** , Introductory Organic Chemistry I
  - Computational Lab TA (2 sessions)
- **CHM247**, Introductory Organic Chemistry II
  - Computational Lab TA