Cher-Tian Ser

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Google Scholar
LinkedIn

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 (Honors) 2015 - 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

Languages

Native
English

Working Proficiency
Mandarin Chinese

Elementary
Korean, French, Danish, German

Publications

7. 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)
6. 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.
5. 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.
4. **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
3. **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
2. **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.
1. Ang, S. J.; **Ser, C. T.**; Wong, M. W., Modeling halogen bonding with planewave density functional theory: Accuracy and challenges, *Journal of Computational Chemistry*, **2019**, *40*, 1829.

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 Methods for Prediction of Corrosion Inhibition Efficiency in Organic Compounds (Poster)

Selected Awards

- **Aug 2019, National Science Scholarship (PhD), A*STAR** (declined)
- **Jul 2019, Lijen Industrial Development Medal, NUS**
  - Awarded for best academic project (Honours Thesis in Chemistry)
- **May 2019, President's Honour Roll, USP**
  - Awarded to USP students with excellence in intellectual and leadership qualities
- **May 2019, Best Performing Student in Sciences and Technology Domain, USP**
- **May 2019, Science Dean's List, NUS**
- **May 2018, Science Dean's List, NUS**
- **Jan 2018, A*STAR Undergraduate Scholarship**

Work Experience

Agency for Science, Technology and Research (A*STAR) Singapore
Materials Science and Chemistry, Institute of High Performance Computing Sep 2019 - Sep 2020
Research Engineer

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