Cher Tian Ser

chertianser.github.io
ctser@cs.toronto.edu

Research Interests

Computational chemistry methods for developing catalytic and energy materials, applied to machine learning methods for high-throughput virtual screening

Publications

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**
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, 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)

Education

University of Toronto — Toronto, Canada
Doctor of Philosophy (Direct Entry) — sep 2020 - present
Chemistry

- Supervised by Prof. Alán Aspuru-Guzik

National University of Singapore — Singapore
Bachelor of Science (Honors) (Highest Distinction) — aug 2015 - jun 2019
Major in Chemistry with a Specialisation in Materials Chemistry

- GPA: 4.77/5.00
- Thesis: *Machine learning methods in modelling corrosion inhibition efficiency of organic compounds* (supervised by Prof. Richard M. W. Wong)
- Minor in Nanoscience
- University Scholars Programme (Honors College)
- Student Exchange Programme to KAIST, South Korea (GPA 4.06/4.30)

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**
- **May 2017, Senior Honour Roll, USP**
- **May 2016, Honour Roll, USP**
- **Dec 2011, Bronze Medal, Singapore Chemistry Olympiad**

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

National University of Singapore Singapore
Department of Chemistry jun 2019 - aug 2019
Research Assistant

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

Skills and Proficiencies

Computational Materials	VASP, Quantum Espresso
Quantum Chemistry	Gaussian, ORCA, Q-Chem
High-Throughput Computing	pymatgen, atomate
Programming Languages	Python, Bash, R, MATLAB, LaTeX
Natural Languages	English (native), Mandarin (working) Korean (elementary), French (elementary)

Co-Curricular Activities and Leadership

USP Tchoukball Club, NUS
Member mar 2018 - jun 2019
Vice-Captain mar 2016 - mar 2018

- Team-bonding, training and member development for more than twenty members
- Represented the faculty and college in competitions
- Achieved Bronze Medal, 2019 Tchouk Cup, and Silver Medal, 2016 Inter-College Games

University Scholars Club, NUS
House Captain sep 2015 - sep 2016

- Head of House Committee; delegating roles and executing efforts for welfare initiatives
- Focused on developing social safety net within college