# 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.

# 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

#### 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.

# 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

# **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

#### Languages

Native Working Proficiency Elementary

English Mandarin Chinese Korean, French, Danish, German