

NEO NENG KAI NIGEL

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WORK EXPERIENCE

DSO National Laboratories

Oct 2023 – Present

Scientist (Member of Technical Staff)

Singapore, Singapore

- As a Data Scientist, I structured problems to be exploited by AI, analysed current AI trends for materials and communicating and visualised results to upper management
- Led research project on inverse design for materials processing, implementing generative AI tools for microstructural generation and characterisation with verification through physics-based models
- Designed and built systems from scratch for data-driven approaches to material design, integrating experience from experimentalists, resulting in optimisation of process workflow with time savings of 55%

EDUCATION

Georgia Institute of Technology

Aug 2022 – Aug 2023

Master of Science in Computer Science (GPA: 4.0/4.0)

Atlanta, Georgia, USA

- Specialisation: Machine Learning (with research project option)

National University of Singapore

Aug 2018 – May 2022

Bachelor of Science (Honours) in Chemistry & Computer Science (CAP: 4.81/5.00)

Singapore

PUBLICATIONS

Towards Fair Graph Anomaly Detection: Problem, New Datasets, and Evaluation

CIKM'24

Neng Kai Nigel Neo, Yeon-Chang Lee, Yiqiao Jin, Sang-Wook Kim, Srijan Kumar

Boise, Idaho, USA

- Full paper published at Conference on Information and Knowledge Management (CIKM) 2024 ([paper](#), [slides](#)).
- We curated novel, real-world datasets to measure fairness in graph anomaly detection methods, and implemented new methods integrating knowledge from fairness and anomaly detection domains with a benchmark for reproducibility.

TALKS / PRESENTATIONS

Lindau Nobel Laureate Conference 2022

June 2022

Panelist - Artificial Intelligence in Chemistry

Lindau, Bavaria, Germany

- Discussed current ideas and future directions in artificial intelligence in chemistry with Nobel Laureates Arieh Warshel and Michael Levitt. Article available at tinyurl.com/lindau2022nigel, with video at tinyurl.com/lindau2022nigelpanel

RESEARCH EXPERIENCE

Georgia Institute of Technology - CLAWS Lab

Dec 2022 – Dec 2023

Graduate Research Assistant // Affiliate

Atlanta, Georgia, USA

- Attached to [Prof Srijan Kumar](#)'s lab for master's research on fair graph anomaly detection - refer to publication above

National University of Singapore - Computational Chemistry Research Lab

Jun 2021 – May 2022

Honours Year Research Student

Singapore

- Attached to [Prof Wong Ming Wah Richard](#)'s lab for honours year research project
- Modified state-of-the-art machine learning models for chemistry (Molecule Attention Transformer) to predict sensitivity values of energetic materials from their molecular structure
- Evaluated tradeoffs using easier to calculate Gasteiger charges instead of calculating from Density Functional Theory
- Investigated how attention matrices in the Transformer model can be used to explain predictions in a chemical context

DSO National Laboratories - Information Department

Jan 2018 – Jun 2018 // May 2020 – Aug 2020

Research Intern

Singapore

- Worked on the inverse problem of reconstructing chemical molecules from mass spectrometer data. Published a paper ([Chemical Structure Elucidation from Mass Spectrometry by Matching Substructures](#)) at [NIPS 2018 Workshop](#)
- Under [Dr Chieu Hai Leong](#), reframed the task as a Reinforcement Learning problem, incorporating Graph Neural Networks using PyTorch Geometric and used Imitation Learning methods to jumpstart learning

SCHOLARSHIPS / AWARDS

DSTA Scholarship

Aug 2018 – Aug 2023

- Sponsorship of undergraduate studies and masters program

Updated as of 2024-12-28. Work authorisation: eligible for the non-lottery [H-1B1 visa](#) (separate quota from H-1B pool)