Sichao Li

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Education Background

- **2021---Present/Australia National University(ANU)/Canberra/Australia**
  - Computational Science/PhD Candidate
- **2018---2020/Australia National University(ANU)/Canberra/Australia**
  - Computer Science/Master/GPA:6.3/7.0

Research Experience

PhD with primary supervisor Prof. Amanda Barnard --- Design-driven Materials Intelligence

[Australian National University, Canberra] 2021.04 --- present

- Designing an interactive and interpretable workflow that predicts a two-way relationship between structures and applications of materials
- Proposing an inverse design workflow for nanoparticles using multi-target machine learning

Research Assistant with supervisor Dr. Charles Martin --- Generating complex melodies on an Edge TPU

[Australian National University, Canberra] 2020.2 --- 2020.7

- Deploying a Recurrent Neutral Network on an Edge TPU and making it work
- Exploring the potential business use with the Dev Board, which contains the Edge TPU

Research Assistant with supervisor Pro. Steve Blackburn --- The Dacapo Bench

[Australian National University, Canberra] 2019.3 --- 2019.12

- Building Dacapo Benchmark on the latest version of JDK
- Testing all benchmarks on MAC, Linux, Windows systems
- Refactoring the Dacapo webpage and maintaining it up-to-date

Services

Course Convenor

[Australian National University, Canberra] 2023.10 --- 2023.12

- Visiting for teaching Data Structure at Shandong University (Weihai Campus)

Academic Tutor

[Australian National University, Canberra] 2019.7 --- present

- Computer Vision, with supervisor Dr. Miaomiao Liu, S1, 2022; S1, 2023
- Foundations of Computing, with supervisor Dr Dirk Pattinson, S2, 2019; S2, 2022
- Relational Database, with supervisor Dr. Lin Yu, S2, 2022; S2, 2023; S1 2024
- Introduction to Database Concepts, with supervisor Dr. Qing Wang, S1, 2023

Journal & Conference Reviewer

[Australian National University, Canberra] 2021.11 --- present

- ICML; Neurips; ICLR; IJCNN; AISTATS; Cell reports Physical Science; Scientific Report

Awards and Scholarships

2021---2024 PhD scholarship at ANU
2018---2019 Summer research scholarship at ANU
2023---2024 International Teaching Fellowship
2024---2025 Vice Chancellor's HDR Travel Grant

Selected Publications

[1] Li, S., & Barnard, A. S. (2022). Inverse design of MXenes for high-capacity energy storage materials using multi-target machine learning. *Chemistry of Materials*, 34(11), 4964-4974.
[2] Li, S., & Barnard, A. S. (2022). Safety-by-design using forward and inverse multi-target machine learning. *Chemosphere*, *303*, 135033.
[3] Li, S., & Barnard, A. (2023, June). Variance Tolerance Factors For Interpreting All Neural Networks. In 2023 International Joint Conference on Neural Networks (IJCNN) (pp. 1-9). IEEE.
[4] Li, S., & Barnard, A. S. (2023). Multi-target neural network predictions of MXenes as high-capacity energy storage materials in a Rashomon set. *Cell Reports Physical Science*, *4*(11).
[5] Li, S., Wang, R., Deng, Q., & Barnard, A. (2024). Exploring the cloud of feature interaction scores in a Rashomon set. *ICLR2024*.
[6] Li, S., Barnard, A. S., & Deng, Q. (2024). Practical Attribution Guidance for Rashomon Sets. *arXiv preprint arXiv:2407.18482*.
[7] Li, S., & Barnard, A. (2024 pre-accepted). Diverse Explanations from Data-driven and Domain-driven Perspectives for Machine Learning Models. *Machine Learning: Science and Technology*.
[8] Li, S., Wang, Xin., & Barnard, A. (2024) EXAGREE: Towards Explanation Agreement in Explainable Machine Learning. *Preprint arxiv.org/abs/2411.01956.*