

Sichao Li

PhD Candidate

Australian National University

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Education Background

- ◆ Australia National University (ANU)/Canberra/Australia 2021.4---2025.4
 - **Ph.D. in Computational Science**
 - Thesis: "Design-driven Materials Intelligence" (Supervisor: Prof. Amanda Barnard)
- ◆ Australia National University (ANU)/Canberra/Australia 2018.7---2020.12
 - **M.Sc. in Computer Science**
 - GPA:6.3/7.0
- ◆ Shanghai Ocean University (SHOU)/Shanghai/China 2014.9---2018.6
 - **B.Eng. in Mechanical Engineering**
 - Recipient of National Scholarship

Research Experience

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

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

- AI for Science (AI4Sci): designing an interactive, inversible, and interpretable workflow that predicts a two-way relationship between structures and applications of materials
- Explainable AI (XAI): studying a set of well-performing models (Rashomon set) and addressing explanation disagreement problem by identifying stakeholder-aligned models
- Produced conference papers in machine learning and scientific journals in physical areas

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 Neural 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

Academic 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 --- 2024.12

- 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

- Introduction to Database Concepts, with supervisor Dr. Qing Wang, S1, 2023
- Research Output: Published several peer-reviewed papers in both leading journals and presented at top-tier ML conferences.

Research Supervision

[Australian National University, Canberra]

2024.02 --- 2024.11

- Supervising Advanced Master of Computing student's final year project
- Project focuses on "Molecular Representation and Regional Explanation", providing expertise in domain knowledge and project management

Academic Reviewer

- Conference Reviewer: ICML, NeurIPS, ICLR, IJCNN, AISTATS
- Journal Reviewer: Cell Reports Physical Science, Scientific Reports

Awards and Scholarships

2018---2019 Summer research scholarship at ANU

2021---2024 PhD scholarship at ANU

2023---2024 International Teaching Fellowship at ANU

2024---2025 Vice Chancellor's HDR Travel Grant at ANU

First Author Publications

Peer-reviewed:

- [1] Li, S., Wang, X., & Barnard, A. (2024). Diverse Explanations From Data-Driven and Domain-Driven Perspectives in the Physical Sciences. *Machine Learning: Science and Technology*.
- [2] Li, S., Wang, R., Deng, Q., & Barnard, A. (2024). Exploring the cloud of feature interaction scores in a Rashomon set. *International Conference on Learning Representations (ICLR)*.
- [3] Li, S., & Barnard, A. (2023). Multi-target neural network predictions of MXenes as high-capacity energy storage materials in a Rashomon set. *Cell Reports Physical Science*.
- [4] Li, S., & Barnard, A. (2023). Variance tolerance factors for interpreting all neural networks. In *2023 International Joint Conference on Neural Networks (IJCNN) (pp. 1-9)*. IEEE.
- [5] 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.
- [6] Li, S., & Barnard, A. (2022). Inverse Design of Nanoparticles Using Multi-Target Machine Learning. *Advanced Theory and Simulations*, 5(2), 2100414.
- [7] Li, S., & Barnard, A. (2022). Safety-by-design using forward and inverse multi-target machine learning. *Chemosphere*, 303, 135033.
- [8] Li, S., Ting, J. Y. C., & Barnard, A. (2022). The impact of domain-driven and data-driven feature selection on the inverse design of nanoparticle catalysts. *Journal of Computational Science*, 65, 101896.
- [9] Li, S., Ting, J. Y. C., & Barnard, A. (2022). Optimization-free inverse design of high-dimensional nanoparticle electrocatalysts using multi-target machine learning. *International Conference on Computational Science*, 307-318.

Preprints:

- [10] Li, S., Barnard, A., & Deng, Q. (2024). Practical Attribution Guidance for Rashomon Sets. *Preprint*.
- [11] Li, S., Deng, Q., & Barnard, A. (2024). EXAGREE: Towards Explanation Agreement in Explainable Machine Learning. *Preprint*.