

Shuya Yamazaki

Curriculum vitae (6th June 2026)

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EDUCATION

Nanyang Technological University

Doctor of Philosophy (PhD) in Materials Science and Engineering

Singapore

Jan. 2025 – Present

Provost Graduate Scholar

Agentic Discovery of Solid-State Inorganic Materials; supervisor: Prof. Kedar Hiappalgaonkar

Nanyang Technological University

Bachelor of Engineering (Hons) in Materials Science and Engineering

Singapore

Aug. 2021 – Dec 2024

NTU President Research Scholar, Best Thesis Award, Accelerated Bachelor Program

Property-directed Generative Design of Inorganic Materials; supervisor: Prof. Kedar Hiappalgaonkar

EXPERIENCE

Institute for Functional Intelligent Materials (I-FIM), NUS

Research Assistant

Singapore

May. 2024 – Dec. 2024

- Conducted research under Prof. Sir Kostya S. Novoselov, Prof. Andrey Ustyuzhanin, and Dr. Nikita Kazeev, contributing to *WyckoffTransformer*, an autoregressive transformer for space group-constrained inorganic crystal structure generation, particularly by enforcing its space group invariance.
- Established S.S.U.N. and Wyckoff template-based novelty benchmarks for evaluating validity, uniqueness, and novelty in crystal structure generation.

Institute of Materials Research and Engineering (IMRE), A*STAR

Research Engineer

Singapore

Jul. 2023 – Dec. 2023

- Co-developed *WyCryst*, the first space group symmetry-aware generative model for inorganic crystal structures based on variational autoencoders.
- Designed Wyckoff position-based crystal representations to incorporate crystallographic symmetry constraints into deep generative modeling.

Materials by Design Lab, NTU

Research Assistant

Singapore

Aug. 2022 – Dec. 2024

- Conducted research under Prof. Kedar Hiappalgaonkar on generative inverse design of inorganic materials.
- Implemented Fourier-transformed crystal representations for inorganic crystal structure generation.
- Developed a multi-property-directed crystal generative model conditioned on formation energy, dynamic stability, space group, and band gap.

PUBLICATIONS

- S. Yamazaki**, Y. Huang, M.H. Petersen, W. Nong, K. Hiappalgaonkar. *Navigating Order-(Dis)Order Family Trees via Group-Subgroup Transitions*. Workshop on AI for Science at the Forty-Third International Conference on Machine Learning (ICML), 2026. arXiv: [2604.21386](https://arxiv.org/abs/2604.21386)
- Z. Wang[†], **S. Yamazaki**[†], M.H. Petersen[†], M. Ohnishi, T. Yamamoto, ..., Z. Ren, J. Shiomi, K. Hiappalgaonkar. *Fast and Accurate Prediction of Lattice Thermal Conductivity via Machine Learning Surrogates*. Submitted. arXiv: [2605.11610](https://arxiv.org/abs/2605.11610)
- Y. Huang, W. Nong, **S. Yamazaki**, M.H. Petersen, J. Wang, R. Zhu, K. Hiappalgaonkar. *SWORD: Symmetry and Wyckoff-sequence of Ordered and Disordered crystals*. Manuscript in preparation. arXiv: [2604.17994](https://arxiv.org/abs/2604.17994)
- S. Yamazaki**[†], W. Nong[†], R. Zhu[†], K.S. Novoselov, A. Ustyuzhanin, K. Hiappalgaonkar. *Multi-property directed generative design of inorganic materials through Wyckoff-augmented transfer learning*. Under review. arXiv: [2503.16784](https://arxiv.org/abs/2503.16784)
- N. Kazeev, W. Nong, I. Romanov, R. Zhu, A. Ustyuzhanin, **S. Yamazaki**, K. Hiappalgaonkar. *WyckoffTransformer: Generation of Symmetric Crystals*. The Forty-Second International Conference on Machine Learning (ICML), 2025. arXiv: [2503.02407](https://arxiv.org/abs/2503.02407)
- R. Zhu, W. Nong, **S. Yamazaki**, and K. Hiappalgaonkar. *WyCryst: Wyckoff inorganic crystal generator framework*. Matter, 2024. DOI: [10.1016/j.matt.2024.05.042](https://doi.org/10.1016/j.matt.2024.05.042)

PRESENTATIONS & CONFERENCES

1. **S. Yamazaki**, Y. Huang, M.H. Petersen, W. Nong, K. Hippalgaonkar. *Autoregressive Transformer for Disordered Crystal Generation*. MRS Spring Meeting & Exhibit, MT03: Atomistic and Generative Modeling for Materials Chemistry and Closed-Loop Design, 2026. **Oral presentation**.
2. A. Dembitskiy, **S. Yamazaki**, A. Maevskiy, N. Kazeev, R.A. Eremin, S. Budenny, K. Hippalgaonkar, A.H.C. Neto, A.E. Ustyuzhanin. *Generative Pipeline for Discovering Solid-State Battery Materials with Universal Atomistic Potentials*. The 25th International Conference on Solid State Ionics (SSI), 2026. **Oral presentation**; Workshop on AI for Science at the Forty-Third International Conference on Machine Learning (ICML), 2026.
3. **S. Yamazaki**, Z. Ren, M.H. Petersen, H. Dai, K. Hippalgaonkar. *CSX Framework for Synthesis-Oriented Generative Materials Discovery*. AI4X-Accelerate Conference, 2026.
4. **S. Yamazaki**[†], W. Nong[†], R. Zhu[†], K.S. Novoselov, A. Ustyuzhanin, K. Hippalgaonkar. *Multi-property directed generative design of inorganic materials through Wyckoff-augmented transfer learning*. AI4X Conference, 2025.

HONOURS & AWARDS

- **Provost Graduate Award**, NTU Singapore. Prestigious university fellowship awarded by the NTU Provost to outstanding PhD students for exceptional academic excellence and demonstrated research potential, with four years of full tuition support and a competitive stipend.
- **Best Final Year Thesis Award**, NTU Singapore. Awarded for the best B.Eng. thesis in the School of Materials Science and Engineering, supervised by Prof. Kedar Hippalgaonkar.