Shuya Yamazaki

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EDUCATION

Nanyang Technological University, Singapore
Doctor of Philosophy (PhD) in Materials Science Jan 2025 – Present

- *NTU Provost Graduate Scholar*
- Research Advisor: Prof. Kedar Hippalgaonkar

Bachelor of Engineering (Hons) in Materials Engineering Aug 2021 – Dec 2024

- *NTU President Research Scholar*
- Accelerated Bachelor Programme with a Specialization in Materials and Artificial Intelligence
- Research Advisor: Prof. Kedar Hippalgaonkar
- Thesis: Property-directed Generative Design of Inorganic Materials

RESEARCH EXPERIENCE

Kedar Hippalgaonkar's Materials by Design Lab, NTU Singapore
PhD student Jan 2025 – Present

- Conducting end-to-end generative design and testing of functional inorganic materials to accelerate discovery of high-performance thermoelectric materials and beyond.
- Submitted a conference paper as the first author to *AI4X 2025 (accepted)*

Final Year Project (FYP) – URECA Jan 2024 – Dec 2024

- Developed Wyckoff-based data augmentation combined with transfer learning to improve the accuracy of material property prediction and multi-property-directed generation of novel inorganic materials
- Submitted a full paper as the first author to *Nature Communications (under review)*

Undergraduate Research Experience on Campus (URECA) Aug 2022 – Jun 2023

- Implemented an invertible crystallographic representation for generative design of inorganic crystals with targeted properties
- Fine-tuned a Variational Auto-Encoder (VAE) to generate inorganic materials with desired mechanical properties, using TensorFlow and scikit-learn

NUS Institute for Functional Intelligent Materials (I-FIM), Research Assistant May 2024 – Dec 2024

- Integrated space group symmetry into autoregressive generative models and established a novel, standardized benchmark to uniformly evaluate and compare generative models for inorganic materials discovery.
- Submitted a conference paper as the co-author to AI4Mat-*NeurIPS-2024 (accepted)*

Agency for Science, Technology and Research (A*STAR) July 2023 – Dec 2023
Institute of Materials Research and Engineering (IMRE), Research Assistant

- Worked on a deep learning algorithm to featurize inorganic materials and employed a Property-directed Variational Auto-Encoder (PVAE) to generate physics-aware crystal structures that preserve space group site symmetry
- Submitted a full paper as the co-author to *Matter (accepted)*

MI-6 Ltd. May 2022 – Jul 2022
Data Science Department, Research Intern

- Deployed a semi-supervised learning framework for quantitative structure-property regression modeling to predict the activity of previously unmeasured novel compounds using SMILES and RDKit
- Performed data processing, analytics and visualization, using Python libraries including NumPy, pandas, scikit-learn, matplotlib and seaborn

SKILLS

Technical: C, C++, Java, Python, TensorFlow, PyTorch, GitHub, CAD, FEM, VESTA, ATOMS
Knowledge: Data Structures, Algorithms, Database, Machine Learning, Generative Models, Materials Science
Language: English, Japanese
Research Interest: Generative Design of Inorganic Materials, Multi-Objective Optimization, Self-Driving Labs

PUBLICATIONS

S. Yamazaki, W. Nong, R. Zhu, KS. Novoselov, A. Ustyuzhanin, K. Hippalgaonkar. “Multi-property directed generative design of inorganic materials through Wyckoff-augmented transfer learning” ***accepted at AI4X 2025***

H. Dai, A. P. Chen, **S. Yamazaki**, A. K. Y. Low, J. Recatala-Gomez, M. Fanxu, K. Hippalgaonkar. “Metastable Polymorph Stabilization with Physics-based Descriptor Engineering and Machine Learning” ***accepted at AI4X 2025***

R. Zhu, W. Nong, **S. Yamazaki**, K. Hippalgaonkar. “WyCryst: Wyckoff Inorganic Crystal Generator Framework”. ***Matter*** 7, 1-20 (2024). https://doi.org/10.1016/j.matt.2024.05.042

N. Kazeev, R. Zhu, I. Romanov, A. Ustyuzhanin**, S. Yamazaki**, W. Nong, K. Hippalgaonkar. “WyckoffTransformer: Generation of Symmetric Crystals” ***accepted at AI4Mat-NeurIPS 2024***

AWARDS & ACHIEVEMENTS

NTU Provost Graduate Award

- Prestigious fellowship awarded by the NTU Provost to the outstanding PhD students for exceptional academic excellence and demonstrated research potential; includes full tuition coverage and a four-year stipend.

NTU President Research Scholar (Distinction)

- In recognition of commendable research accomplishments with Distinction in URECA Undergraduate Research Programme