

Hyuk Jun Yoo

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BRIEF INTRODUCTION

I hold a Ph.D., specializing in autonomous laboratories for materials discovery in South Korea, where my experiences span a broad spectrum from hardware construction to software development. This includes hardware module design, experiment planning, operating system, computer vision, and web crawling for autonomous laboratories. My research interests focus on AI model development, lab automation, operating system (orchestration software), and AI-driven material discovery.

EXPERIENCES

- 2025.08 -**
 - Postdoctoral Researcher
 - Material Science and Engineering in UC Berkeley & LBNL
 - Advisor: Prof. Gerbrand Ceder
- 2025.03 -**
 - Postdoctoral Researcher
- 2025.08**
 - Korea Institute of Science and Technology (KIST)
 - Advisor: Dr. Sang Soo Han

EDUCATION

- 2020.03-**
 - M.S. & Ph.D. in Department of Chemical and Biological Engineering
- 2025.02**
 - Korea Institute of Science and Technology (KIST)
 - Korea University
 - *Thesis: Autonomous Laboratory for Metal Nanoparticles Synthesis*
 - Advisor: Dr. Sang Soo Han, Prof. Kwan-Young Lee
 - Cumulative GPA: 4.11/4.50 | GPA (100-point scale): 95.5
- 2013-2020**
 - B.S. Department of Applied Chemistry
- (2015-2016:
Military Service)
 - Kyung Hee University, Yongin.
 - Cumulative GPA: 4.00/4.50 | GPA (100-point scale): 94.3

SKILLS

Professional skills (* text represents a high-level skills)

AI optimization	Python* , Scikit-learn* , Pytorch*
Hardware	Arduino* , Fusion360* , Socket* , TCP/IP protocol* , Linux* , Robotic arm* , ROS
Interface & Crawling	HTML* , CSS, JavaScript, BeautifulSoup* , Selenium*
Experiment	Metal nanoparticle synthesis* , Image analysis of SEM, TEM
Data management	MongoDB* , JSON, Sharding

RESEARCH INTERESTS

- AI model development for experiment planning
- Lab automation & Computer vision in chemistry lab
- Operating system for autonomous laboratory (Orchestration software)
- Nanomaterial design, Material discovery, Drug discovery

PUBLICATIONS LIST

Publications († = Equal contribution)

Jun 2024

OCTOPUS: Operation Control System for Task Optimization and Job Parallelization via a User-Optimal Scheduler



Yoo, H. J., Lee, K-Y., Kim, D. and Han, S. S., *Nature Communications* (2024), **15**, 9669

- Conceptualization of multi-user system with user-optimal scheduler
- Development of OCTOPUS's architecture
- Development of scheduling system

Feb 2024

Bespoke Metal Nanoparticle Synthesis at Room Temperature and Discovery of Chemical Knowledge on Nanoparticle Growth via Autonomous Experimentations.



Yoo, H. J.[†], Kim, N.[†], Lee, H., Kim, D., Ow, L. T. C., Nam, H., Kim, C., Lee, S. Y., Lee, K-Y., Kim, D. and Han, S. S., *Advanced Functional Materials* (2024), **34**, 2312561 –

Selected as Front Cover Image

- Conceptualization of chemical knowledge discovery in accumulated datasets
- Development of batch synthesis module and UV-Vis module
- Development of Bayesian optimization with early stopping

- Analysis of TEM image and UV-Vis spectrum
- SHAP analysis and Chemical knowledge discovery

Feb 2024

Machine Vision-based Detections of Transparent Chemical Vessels Toward the Safe Automation of Material Synthesis.



Tiong, L. C. O.[†], **Yoo, H. J.[‡]**, Kim, N., Kim, C., Lee, K. Y., Han, S. S., & Kim, D., *npj Computational Materials* (2024), **10** (1), 42

- Conceptualization of safety issues
- Development of DenseSSD vis deep learning approach
- Case studies of safety issues in autonomous laboratories

Manuscripts in preparation († = Equal contribution)

1. **Yoo, H. J.**, Lee, K-Y., Kim, D. and Han, S. S. (in prep) Synthesis Order/Condition Simultaneous Optimization for Bespoke Nanoparticle Synthesis via Autonomous Experimentations
2. Kim, N.[†], **Yoo, H. J.[‡]**, Lee, K-Y., Kim, D. and Han, S. S. (in prep). AI-based Exploration on Synthesizable Space for Autonomous Laboratory

PRESENTATIONS

International presentations († = Equal contribution)

Feb 2025

[Poster] **Yoo, H. J.**, D.Kim, Han, S. S. "Unlocking the Potential of Synthesis Order for Bespoke Nanoparticles via Autonomous Laboratory", *2025 Nature Conference. AI for Materials, Materials for AI*

Nov 2024

[Oral] **Yoo, H. J.[‡]**, Kim, N.[†], Lee, H., Kim, D., Ow, L. T. C., ... & Han, S. S. "Autonomous Laboratory for Bespoke Metal Nanoparticle Synthesis and Chemical Knowledge Discovery, *2024 International Conference on Electronic Materials and Nanotechnology for Green Environment (ENGE)*

Oct 2024

[Oral] **Yoo, H. J.[‡]**, Kim, N.[†], Lee, H., Kim, D., Ow, L. T. C., ... & Han, S. S. "Bespoke Metal Nanoparticle Synthesis and Chemical Knowledge Discovery via Autonomous Experimentations", *2024 AIChE Fall Meeting*

- July 2023** [Poster] Yoo, H. J.[†], Kim, N.[†], Lee, H., Kim, D., Ow, L. T. C., Nam, H., ... & Han, S. S. "Chemistry Discovery in Nanoparticle Synthesis via Autonomous Laboratory", 2023 *Nanokorea*
- Nov 2022** [Poster] Yoo, H. J.[†], Kim, N.[†], Kim, D., & Han, S. S. "Autonomous Laboratory for Bespoke Synthesis of Nanoparticles", 2022 *MRS Fall meeting*
- Nov 2022** [Poster] Yoo, H. J.[†], Kim, N.[†], Lee, H., Kim, D., Ow, L. T. C., Nam, H., ... & Han, S. S. "AI-Robotics Based Bespoke Synthesis Planning of Ag Nanoparticle, Automation vs Autonomy", 2022 *International Conference on Electronic Materials and Nanotechnology for Green Environment (ENGE)*

Domestic presentations († = Equal contribution)

- May 2025** [Oral] Yoo, H. J. "AI-Robotics Based Autonomous Laboratory for Novel Material Discovery", *Graduate Seminar in Kyung Hee University*
- Apr 2025** [Oral] Yoo, H. J., D.Kim, Han, S. S. "Unlocking the Potential of Synthesis Order for Bespoke Nanoparticles via Autonomous Laboratory", 2025 *Spring Conference of the Korean Institute of Metals and Materials*
- Feb 2025** [Oral] Yoo, H. J. "Autonomous Laboratory Leading Future R&D Innovation", *Council for AI Drug Discovery and Development*
- Oct 2024** [Oral] Yoo, H. J.[†], Kim, N.[†], Lee, H., Kim, D., Ow, L. T. C., ... & Han, S. S. "Bespoke Metal Nanoparticle Synthesis and Chemical Knowledge Discovery via Autonomous Laboratory", 2024 *KICChE Fall Meeting*
- Apr 2024** [Oral] Yoo, H. J.[†], Kim, N.[†], Lee, H., Kim, D., Ow, L. T. C., ... & Han, S. S. "Bespoke Metal Nanoparticle Synthesis at Room Temperature and Discovery of Chemical Knowledge on Nanoparticle Growth Via Autonomous Experimentations", 2024 *KICChE Spring Meeting*
- Apr 2023** [Oral] Yoo, H. J.[†], Kim, N.[†], Lee, H., Kim, D., Ow, L. T. C., ... & Han, S. S. "Chemistry Understanding and Discovery in Bespoke Nanoparticle Synthesis via Autonomous Laboratory with Early Stopping", 2023 *Spring Conference of the Korean Institute of Metals and Materials*

HONORS AND AWARDS

Feb 2025	[Award] 2024 KU Achievement Award (Summa Cumme Laude), <i>Korea University</i>
Feb 2025	[Award] Outstanding Graduate Students Award (Summa Cumme Laude), <i>2024 KIST Scholarship</i> *This scholarship was the biggest competition between graduated students in KIST (\$300)
Nov 2024	[Oral] Best Award, <i>2024 International Conference on Electronic Materials and Nanotechnology for Green Environment</i> Title: “Autonomous Laboratory for Bespoke Metal Nanoparticle Synthesis and Chemical Knowledge Discovery”
Aug 2024	[Scholarship] Best Performance Award, <i>2024 KIST Scholarship</i> *This scholarship was the biggest competition between graduated students in KIST (\$3,000)
Apr 2024	[Oral] Best Award, <i>2024 Spring Conference of the KICChE Spring Meeting</i> Title: “Bespoke Metal Nanoparticle Synthesis at Room Temperature and Discovery of Chemical Knowledge on Nanoparticle Growth via Autonomous Experimentations”
Aug 2023	[Poster] Best Award, <i>2023 Nanokorea</i> Title: “Chemistry Discovery in Nanoparticle Synthesis via Autonomous Laboratory”
Apr 2023	[Oral] Best Award, <i>2023 Spring Conference of the Korean Institute of Metals and Materials</i> Title: “Chemistry Understanding and Discovery in Bespoke Nanoparticle Synthesis via Autonomous Laboratory with Early Stopping”
Nov 2022	[Poster] Best Award, <i>2022 International Conference on Electronic Materials and Nanotechnology for Green Environment</i> Title: “AI-Robotics Based Bespoke Synthesis Planning of Ag Nanoparticle, Automation vs Autonomy”

REFERENCES

- Dr. Sang Soo Han
- Principal Research Scientist
 - Computational Science Research Center, KIST, Korea
 - 5 Hwarangno 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea
 - Email: sangsoo@kist.re.kr

**Dr. Sang Soo Han was my supervisor during my Ph.D. course at KIST.*

- Prof. Kwan-Young Lee
- Professor
 - Department of Chemical and Biological Engineering, Korea University, Korea
 - 145, Anam-ro, Seongbuk-gu, Seoul, Republic of Korea
 - Email: kylee@korea.ac.kr

**Prof. Kwan-Young Lee was my supervisor during my Ph.D. course at Korea University.*

- Dr. Donghun Kim
- Senior Research Scientist
 - Computational Science Research Center, KIST, Korea
 - 5 Hwarangno 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea
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**Dr. Donghun Kim was my advisor during my Ph.D. course at KIST.*

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- Senior Research Scientist
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**Dr. Byungju Lee was my advisor during my Ph.D. course at KIST.*

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