

Hyuk Jun Yoo

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BRIEF INTRODUCTION

I am a graduate student studying an autonomous laboratories for materials discovery in South Korea, where my experiences span a broad spectrum from hardware construction to software development. This includes hardware system 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.

EDUCATION

- 2020-present**
- M.S. & Ph.D. Course Student in Department of Chemical and Biological Engineering
 - 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**
(2015-2016:
Military Service)
- B.S. Department of Applied Chemistry
 - 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

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., Acceptance to *Nature Communications* (2024), <https://doi.org/10.21203/rs.3.rs-4254570/v1>

- 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

- 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 Optimization for Chemical Knowledge Transfer 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 conference presentations († = Equal contribution)

- 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*

Domestic conference presentations († = Equal contribution)

- 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

Aug 2024 [Scholarship] Best Performance Award, *2024 KIST Scholarship*

*This scholarship was the biggest competition between graduated students in KIST (\$3,000)

Apr 2024 [Oral] Best Award, *2024 Spring Conference of the KICChE Spring Meeting*

Title: “Bespoke Metal Nanoparticle Synthesis at Room Temperature and Discovery of Chemical Knowledge on Nanoparticle Growth via Autonomous Experimentations”

Aug 2023 [Poster] Best Award, *2023 Nanokorea*

Title: “Chemistry Discovery in Nanoparticle Synthesis via Autonomous Laboratory”

Apr 2023 [Oral] Best Award, *2023 Spring Conference of the Korean Institute of Metals and Materials*

Title: “Chemistry Understanding and Discovery in Bespoke Nanoparticle Synthesis via Autonomous Laboratory with Early Stopping”

Nov 2022 [Poster] Best Award, *2022 International Conference on Electronic Materials and Nanotechnology for Green Environment*

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
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**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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**Dr. Byungju Lee was my advisor during my Ph.D. course at KIST.*

Update in Oct, 24th, 2024