Hyuk Jun Yoo

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BRIEF INTRODUCTION

I'm a postdoctoral researcher at Lawrence Berkeley National Laboratory (LBNL), specializing in self-driving laboratories (SDL) for material and chemical discovery with a particular focus on adaptive *in-situ* XRD experimentation to reveal hidden intermediate phases. My research interests focus on scientific knowledge discovery with AI and robotics. With extensive experience ranging from lab automation to software development, my expertise includes lab automation design, AI-driven experiment planning, and the development of orchestration software for SDL. Additionally, I have worked on computer vision, web crawling, LLM for material data mining and recipe recommendation.

EXPERIENCES

2025.08 - Current
- Postdoctoral Researcher
- Material Sciences Division in LBNL & Material Science and Engineering in UC Berkeley
- Advisor: Prof. Gerbrand Ceder

2025.03 - 2025.08
- Postdoctoral Researcher
- Korea Institute of Science and Technology (KIST)
- Advisor: Dr. Sang Soo Han

EDUCATION

2020.03- 2025.02
- M.S. & Ph.D. in Department of Chemical and Biological Engineering
  - Korea Institute of Science and Technology (KIST) – *Summa Cumme Laude**
  - Korea University – *Summa Cumme Laude**
- *Thesis: Autonomous Laboratory for Metal Nanoparticle 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

RESEARCH INTERESTS

- Scientific knowledge discovery with AI and robotics
- 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

SKILLS

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

AI optimization	**Python*, Scikit-learn*, Pytorch***
Lab Automation	**Arduino*, Fusion360*, Socket*, TCP/IP protocol*, Linux*, Robotic arm (Universal Robotics, Doosan Robotics, OnRobot, Robotiq)*, Liquid Handler (Tecan, Hamilton)*, Powder Handler (Mettler Toledo)*,** ROS
Experiment	**In-situ XRD*, XRD*, Metal nanoparticle synthesis***, **UV-Vis characterization***, FullProf, GSAS-II, Image analysis of SEM and TEM
Interface & Crawling	**HTML*,** CSS, JavaScript**, BeautifulSoup*, Selenium***
Data management	**MongoDB***, JSON, Data Schema, Pydantic, LIMS, Sharding
Collaboration tools	**Notion*, Slack*, Microsoft* (Word, PowerPoint, Excel), Google* (Drive, Gmail, Calendar), Dooray***

PUBLICATIONS LIST

Publications († = Equal contribution)

Oct 2025 Toward Self-Driving Laboratory 2.0 for Chemistry and Materials Discovery
Lee. H. †, **Yoo. H. J.**‡, Jang. H. S., Park. B. H., Park. Y. J., and Han. S. S., *Materials Horizon (In Press: Materials Horizon)* (2025)

- Conceptualization of review and perspective
- Draft manuscript of perspective and draw future plan for next self-driving labs 2.0
- Review all parts

Jun 2025 *NanoChef*: AI Framework for Synthesis Sequence and Reaction Conditions Simultaneous Optimization via Autonomous Laboratories

Yoo. H. J., Kim. D. Yim. S., and Han. S. S., *ChemRxiv (Revision: Journal of American Chemical Society)* (2025)

- Conceptualization and *NanoChef*
- Development of deep learning-based Bayesian optimization protocol
- Chemical knowledge discovery of Ag nanoparticle varying synthesis order
- Draft manuscript

Jun 2025 You Only Put Your Nanoparticle: A Fully Automated System for Nanoparticle Washing Enabled by Vision and Language AI

Lee. H., Kim. D., Lee. H., Gwak. N., Kim. N., **Yoo. H. J.**, Yu. T., Oh. N., Sohn. S. S., and Han S. S., *ChemRxiv (under review: Chemical Engineering Journal)* (2025)

- Conceptualization and development of washing module
- Comments of workflow and performance analysis for computer vision and LLM
- Comments of main figure

May 2025 SPACESHIP: synthesizable parameter acquisition via closed-loop exploration and self-directed, hardware-aware intelligent protocols for autonomous lab

Kim. N.†, **Yoo. H. J.**‡, Kim. D., Lee. H., and Han. S. S., *ChemRxiv (Revision: Journal of American Chemical Society)* (2025)

- Conceptualization of synthesizable space exploration
- Chemical knowledge discovery of Au nanorod growth mechanism
- Experiment of Au nanorod synthesis
- Analysis of TEM images and UV-Vis spectrum
- Draft manuscript

Jul 2025 Self-Driving Laboratories with Artificial Intelligence: An Overview of Process Systems Engineering Perspective

Kim, Y., Doo, H., Shin, D., Lee, S. Y., Roh, Y., Park, S., ... **Yoo. H. J.** ... & Na, J. (2025). *Computers & Chemical Engineering* (2025), 109266

- Conceptualization and review of OS part
- Draft manuscript

Nov 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 and performance analysis of scheduling system
- Development of supplementary guidelines for researchers
- Draft manuscript

Jul 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., Tiong. L. C. O., 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
- Draft manuscript

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 architecture vis deep learning approach
- Case studies of safety issues in autonomous laboratories
- Draft manuscript

Manuscripts in preparation († = Equal contribution)

1. **Yoo, H. J.**‡, and Gerbrand, Ceder. (in prep) *in-situ* XRD Automatic Operation for Material Phases Identification
2. **Yoo, H. J.**‡, and Gerbrand, Ceder. (in prep) Adaptive *in-situ* XRD Automatic Operation for Hidden Intermediate States

PATENTS

US patents

Sep 2025 *System and method for operating laboratory based on modular experiment process*

Sang Soo Han, Donghun Kim, **Hyuk Jun Yoo**

- Conceptualization of system architecture
- Development of all operational code

Dec 2024 *Modular experiment autonomation system and method of operating the same*

Sang Soo Han, Donghun Kim, **Hyuk Jun Yoo**, Nayeon Kim, Seung Yong Lee

- Conceptualization of modular experiment automation system
- Development of batch synthesis module and UV-Vis module

Nov 2024 *Method and apparatus for diagnosing error of object placement using artificial neural network*

Donghun Kim, Sang Soo Han, Leslie Tiong Ching OW, **Hyuk Jun Yoo**, Nayeon Kim

- Conceptualization of safety issues
- Development of DenseSSD architecture vis deep learning approach

PRESENTATIONS

International († = Equal contribution)

Jan 2026 **[Presentation *(Invited)*]** **Yoo, H. J**., K-Y. Lee, D.Kim, Han, S. S. "OCTOPUS: Operation Control System for Job Parallelization and Task Optimization via User-Optimal Scheduler in Self-Driving Labs", *2026 Orchestration Alignment Virtual Workshop (AC Consortium)*

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 2024 **[Exhibition]** **Yoo, H. J**., Kim, N., Lee, H., Kim, D., Kim, D., and Han, S. S. "AI-Robotics based Bespoke Nanomaterial Synthesis Autonomous Laboratory", *2024 Nanokorea*

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)*

July 2022 **[Poster]** Tiong. L. C. O.†, **Yoo. H. J.**‡, Kim. N., Lee. K. Y., Han. S. S., & Kim. D., "Improving Safety in Autonomous Laboratory via Vial-Positioning Detection using Deep Learning and Computer Vision", *2022 Nanokorea*

Domestic († = Equal contribution)

June 2025	**[Oral *(Invited)*]** **Yoo, H. J**. "Autonomous Laboratory for Metal Nanoparticle Synthesis", *Seminar in Prof. Jonghee Yang Group at Yonsei University*
June 2025	**[Oral *(Invited)*]** **Yoo, H. J**. "Autonomous Laboratory for Metal Nanoparticle Synthesis", *Seminar in Prof. Dong-Hwa Seo Group at Korea Advanced Institute of Science and Technology (KAIST)*
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 *(Invited)*]** **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 KIChE 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 KIChE 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*), *Korea University*

Feb 2025 **[Award]** Outstanding Graduate Students Award (*Summa Cumme Laude*), *2024 KIST Scholarship*

*This scholarship was the biggest competition between graduated students in KIST ($300)

Nov 2024 **[Oral]** Best Award, *2024 International Conference on Electronic Materials and Nanotechnology for Green Environment*

Title: "Autonomous Laboratory for Bespoke Metal Nanoparticle Synthesis and Chemical Knowledge Discovery"

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 KIChE 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"

NEWS

Domestic († = Equal contribution)

Mar 2025 **[Youtube] Demonstration of autonomous lab system for AI-guided synthesis** Interview experimental planning, robotic control, and real-time feedback of autonomous laboratories at *Council for AI Drug Discovery and Development in South Korea*

Nov 2024 **[News, News, News, News] Featured in Yonhap News and other media for the development of a dedicated operating system for autonomous laboratories:** Introduced as a key contributor to an AI-driven orchestration software enabling multi-user, multi-task automation in scientific research environments.

May 2024 **[News] Smart Labs for Bespoke Synthesis of Nanomaterials:** *Recognized for contributions to AI-guided autonomous lab systems enabling closed-loop nanomaterial optimization at KIST.*

Apr 2024 **[Youtube] AI-Robotics Based Autonomous Laboratory for Nanomaterial Discovery:** Featured system demonstration video highlighting my contributions to intelligent experiment planning, real-time control, and automated synthesis workflows. This work showcases scalable infrastructure for AI-driven materials research.

MEMBERS & BOARD

- ✓ *KIChE* (Korea Institute of Chemical Engineering)
- ✓ *KIMM* (Korean Institute of Metals and Materials)
- ✓ *AIChE* (American Institute of Chemical Engineering)
- ✓ *MRS* (Materials Research Society)

REFERENCES

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- 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 and postdoctoral research 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.*

Prof. Gerbrand Ceder
- Chancellor's Professor / Faculty Scientist
- Department of Materials Science and Engineering, UC Berkeley, U.S Materials Sciences Division, Lawrence Berkeley National Laboratory, U.S
- Building 33, Room 142B, Berkeley, CA 94720
- Email: gceder@berkeley.edu

**Prof. Gerbrand Ceder was my supervisor during my postdoctoral research at LBNL.*

Prof. Donghun Kim
- Associate Professor
- Department of Material Science and Engineering, KAIST, Korea
- W1-3307, KAIST, 291 Daehak-ro, Yuseong-gu, Daejeon, Republic of Korea
- Email: donghun.kim@kaist.ac.kr

**Prof. Donghun Kim was my advisor during my Ph.D. course and postdoctoral research at KIST.*

Dr. Byungju Lee
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- Computational Science Research Center, KIST, Korea
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**Dr. Byungju Lee was my advisor during my Ph.D. course and postdoctoral research at KIST.*

Update to Feb 21th, 2026