

# Minjae Kwen

## Curriculum Vitae

Department of Chemistry, KAIST,  
291, Daehak-ro, Yuseong-gu, Daejeon, Republic of Korea(34141)

## Contact Info

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QR code  
directs you to Website:



## Research Interests

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### Computational Chemistry

- Nonadiabatic Dynamics Simulations
- First-principle Calculations in Catalytic Reactions

### Synthesis and Application of Nanocatalysts

## Educations

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### KAIST, Daejeon

Mar. 2019 – Present

*Major in Chemistry (Minor: Material Science)*

- Current GPA: 4.18/4.3, Major GPA: 4.23/4.3
- Military Service, Alternative: May. 2022 – Feb. 2024

### UC Berkeley, Berkeley, CA

Jun. 2019 – Aug. 2019

Summer Sessions at UC Berkeley

### Daegu Science High School, Daegu

Mar. 2016 – Feb. 2019

High school for the gifted in science and mathematics

## Publications

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### Journal Articles

1. *Splitting of Hydrogen Atoms into Proton–Electron Pairs at BaO–Ru Interfaces for Promoting Ammonia Synthesis under Mild Conditions*  
J. Am. Chem. Soc. 2023, 145, 20, 11364–11374.  
: As a co-first author, performed DFT calculation study of BaO–Ru interface in Ba–Ru/MgO catalyst.

### Conference Papers

1. *Time-domain ab initio analysis of facet-dependent carrier dynamics in Cuprous oxide*  
ISTCP 2024, Poster  
: As a first researcher, performed semiclassical nonadiabatic dynamics simulation on carrier recombination

## Research Experiences

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### M-design Lab (KAIST)

Sep. 2021 – Present

*Individual Study, Undergraduate Research Program (URP)*

**Advisor:** Hyungjun Kim

**Topic:**

- Time-domain ab initio analysis of facet-dependent carrier dynamics in Cuprous oxide
- Splitting of Hydrogen Atoms into Proton–Electron Pairs at BaO–Ru Interfaces for Promoting Ammonia Synthesis under Mild Conditions - Computational Study
- Screening Pathways for Nitrogen Monoxide Electroreduction on Transition Metal on TPP using Density-Functional Theory

**Nanocatalyst Research Laboratory (KAIST)**

Apr. 2021 – Aug. 2021

*Individual Study***Advisor:** Hyunjoon Song**Topic:** Synthesis, characterization, and application of various nanocatalysts**Electrochemical Materials Design Laboratory (KAIST)**

Dec. 2020 – Feb. 2021

*Individual Study***Advisor:** Hye Ryung Byon**Topic:** Electrochemical Potential Window of Molecular Crowded Electrolyte with Various Li Salt

## Honors and Awards

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**Overseas PhD Scholarship (Training Program), Chemistry**

2024–Present

*Korea Foundation for Advanced Studies (KFAS)*

Designed to support outstanding PhD students in world's top universities

**Korean Presidential Science Scholarship, Chemistry**

2019–Present

*Korea Student Aid Foundation (KOSAF)*

Designed to support top undergraduates in Korea, about twenty freshmen in chemistry selected annually

**KAIST Presidential Fellowship (KPF)**

2019–Present

*Global Leadership Center, KAIST*

Designed to support top students in KAIST, twenty-six freshmen selected in 2019

**Dean's list, KAIST**

2021

*Department of Chemistry, KAIST*

Best academic performance during the first six semesters, Spring 2019–Fall 2021

## Others

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**Academic Conferences**

2024

- ISTCP 2024, Qingdao, China

Academic conference for theoretical chemical physics, delivered poster presentation

- NANO KOREA 2024, Goyang-si, Republic of Korea

Academic conference specializing in the nanotechnology

- 2024 Korea-Japan Symposium on Molecular Science, Busan, Republic of Korea

Academic conference for cutting-edge molecular sciences

**KAIST-IIT Madras Joint Research Challenge**

2020

*Indian Institute of Technology Madras, Chennai, Tamil Nadu, India*

Collaborated research with IITM students on the topics of sustainable environment

**Alternative Military Service (Social Service)**

2022–2024

*Dangaram Kindergarten, Hanam-si, Gyeonggi-do, Korea*