

# Minjae Kwen

*Curriculum Vitae*

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

## Contact Info

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Email: kmjaday0082@kaist.ac.kr  
Phone: +82-10-9204-6950  
Website: <https://minjaekwen.github.io/>

QR code  
directs you to Website:



## Research Interests

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### Computational Chemistry

- Quantum Nonadiabatic Dynamics Simulations
- First-principle Electronic Structure Calculations (DFT and post-HF methods)

### Electrocatalytic / Photocatalytic reactions

## 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. Baik, Y., Kwen, M. *et al.* Splitting of hydrogen atoms into proton–electron pairs at BaO–Ru interfaces for promoting ammonia synthesis under mild conditions. *Journal of the American Chemical Society* 145.20 (2023): 11364-11374. (Doi: 10.1021/jacs.3c02529.)  
: As a co-first author, performed DFT calculation study of BaO-Ru interface in Ba-Ru/MgO catalyst.

### Conference Papers

1. Kwen, M. *et al.* (2024). Time-domain ab initio analysis of facet-dependent carrier dynamics in Cuprous oxide, ISTCP 2024, Poster ([link](#))  
: 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

**Advisor:** Hyungjun Kim

**Topic:**

- Time-domain ab initio analysis of facet-dependent carrier dynamics in Cuprous oxide [Poster]
- DFT study for separate storage of proton–electron pairs at BaO–Ru interfaces [Published]
- DFT screening study for NO Electroreduction on Transition Metal on TPP

### Nanocatalyst Research Laboratory (KAIST)

Apr. 2021 – Aug. 2021

**Advisor:** Hyunjoon Song

**Topic:** Synthesis, characterization, and application of various nanocatalysts

### Electrochemical Materials Design Laboratory (KAIST)

Dec. 2020 – Feb. 2021

**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
- NANO KOREA 2024, Goyang-si, Republic of Korea
- 2024 Korea-Japan Symposium on Molecular Science, Busan, Republic of Korea

### 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*