Minjae Kwen

Curriculum Vitae

Quantum Science and Engineering, Harvard University,
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Research Interests

Many-Body & Complex Systems
– Quantum statistical / condensed-matter theory
– Complex systems at the chemistry–physics interface

Computational Chemistry
– Nonadiabatic Dynamics (Surface Hopping)
– First–principle Electronic Structure Calculations

Educations

Harvard University, Cambridge, MA 2025 – Present
Ph.D. Student in Quantum Science and Engineering

KAIST, Daejeon 2019 – 2025
B.S in Chemistry (Minor: Material Science)
– Valedictorian (GPA: 4.18/4.3, *Summa Cum Laude*)
– Military Service, Alternative: May. 2022 – Feb. 2024

Daegu Science High School, Daegu 2016 – 2019
High school for the gifted in science and mathematics

Publications

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

M-design Lab (KAIST) Sep. 2021 – Aug. 2025

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

Korean Chemical Society Presidential Award 2025
Korean Chemical Society (KCS)
Awarded to the top academic performer among undergraduate graduates

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 2019–2025
Korea Student Aid Foundation (KOSAF)
Designed to support top undergraduates in Korea, about twenty freshmen in chemistry selected annually

KAIST Presidential Fellowship (KPF) 2019–2025
Global Leadership Center, KAIST
Designed to support top students in KAIST, twenty-six freshmen selected in 2019

Others

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

UC Berkeley, Summer Sessions 2019
UC Berkeley, Berkeley, CA

Alternative Military Service (Social Service) 2022–2024
Dangaram Kindergarten, Hanam-si, Gyeonggi-do, Korea