

Stephanie Kwon, Ph.D.

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EDUCATION

Doctor of Philosophy **2010-2015**

Chemical and Biological Engineering
Northwestern University (Evanston, IL)
Laboratories of Drs. Randall Snurr and Peter Stair
Dissertation: Gas-phase alkene oxidation by hydrogen peroxide: the nature of active oxygen species in heterogeneous catalysis

Bachelor of Science (graduated with *magna cum laude*) **2005-2010**

Chemical and Biological Engineering
Seoul National University (Seoul, Korea)

RESEARCH EXPERIENCE

Postdoctoral Fellow, University of California (UC), Berkeley (PI: Dr. Enrique Iglesia) **2015-**

- Uncovered mechanistic details of O₂ activation routes in Mars-van Krevelen redox cycles by incorporating scavenging experiments with density-functional theory (DFT) calculations.
- Identified descriptors of rates and selectivities of inner and outer sphere O₂ activation pathways using theoretical assessments based on DFT calculations. (*Manuscript in preparation for submission*)
- Elucidated HCOOH decomposition elementary steps on TiO₂ and Cu catalysts using combined efforts of kinetic, isotopic, spectroscopic, and temperature programmed surface reaction experiments and of DFT calculations on the energetics of intermediates and transition stations involved in the plausible reaction routes. Such results revealed unprecedented mono- and bi-molecular routes that change with surface coverages. (*Manuscripts in preparation for submission*)

Ph.D. Student, Northwestern University (PIs: Drs. Randall Snurr and Peter Stair) **2010-2015**

- Revealed the kinetics and elementary steps of gas-phase cyclohexene epoxidation with H₂O₂(g) on titanium silicate-1 (TS-1) catalysts by developing a flow reactor system that utilizes H₂O₂(g).
- Demonstrated propene oxidation with H₂O₂(g) to form acetone on Pd/Al₂O₃ and identified the reaction mechanisms via a detailed kinetic analysis, combined with DFT calculations
- Investigated the effects of basic oxide over-layers on TiO₂ catalysts for CO₂ adsorptions using DFT calculations and demonstrated the enhanced reactivities of MgO-decorated TiO₂ for CO₂ photo-reduction
- Identified O₂ activation routes on the coordinatively unsaturated Co sites in Co-MOF using DFT calculations

Undergraduate Researcher, Seoul National University (PI: Dr. Sang-Heup Moon) **2009-2010**

- Improved the reactivity and stability of LaNiO₃ perovskite catalysts for methane reforming reactions

by supporting them into mesoporous silica. Further characterizations revealed the conversion of the perovskite structures into highly dispersed Ni on La₂O₃ during reactions.

PUBLICATION

1. **Kwon, S.**, P. Deshlahra, and E. Iglesia. (2018) Dioxygen activation routes in Mars-van Krevelen redox cycles catalyzed by metal oxides *J. Cat.*, 364, 228–247.
2. **Kwon, S.**, P. Liao, P. C. Stair P. C, R. Q. Snurr (2016) Alkaline-earth metal-oxide overlayers on TiO₂: application toward CO₂ photoreduction, *Catal Sci Technol.*, 6, 7885–7895.
3. **Kwon, S.**, N. M. Schweitzer, S.Y. Park, P. C. Stair P. C, and R. Q. Snurr (2015) A kinetic study of vapor-phase cyclohexene epoxidation by H₂O₂ over mesoporous TS-1, *J. Cat.*, 323, 117–115.
4. Tuci, G., Giambastiani, G., **Kwon, S.**, Stair, P. C., Snurr, R. Q., and Rossin, A. (2014) Chiral Co(II) metal-organic framework in the heterogeneous catalytic oxidation of alkenes under aerobic and anaerobic Conditions, *ACS Catal.*, 4, 1032–1039.
5. Mondloch, J. E., Bury, W., Fairen-jimenez, D., **Kwon, S.**, Demarco, E. J., Weston, M. H., Sarjeant, A. A., Nguyen, S. T., Stair, P. C., Snurr, R. Q., Farha, O. K., and Hupp, J. T. (2013) Vapor-phase metalation by atomic layer deposition in a metal-organic framework., *J. Am. Chem. Soc.*, 135, 10294–10297 (*Highlighted in Chemical & Engineering News*).

FUNDING

ExxonMobil

2018

Role: Contributed foundational ideas and preliminary data

Amount: \$750,000 - \$250,000 per year (total 3 years)

Energy Frontier Research Center (ERFC), supported by the DOE office (*declined*)

2018

Title: Reactive intermediate-enabled coupling of reactions

Role: Provided preliminary data and wrote a part of the proposal

Startup and production allocation awards from NERSC, supported by the DOE office

2017-2018

Title: Roles of gas-phase molecular shuttles in heterogeneous catalysis

Role: PI proxy

Amount: each 50,000 NERSC core-hours

Production allocation award from XSEDE, supported by NSF

2016-2017

Title: Understanding mechanisms of O₂ activation for selective oxidation reactions by metal oxides

Role: PI

Amount: 1,062,000 core-hours

Startup allocation award from XSEDE, supported by NSF

2016-2017

Title: Selective oxidation of methanol on polyoxometalate clusters

Role: PI

Amount: 50,000 core-hours

HONORS AND AWARDS

- ***Catalysis and Reaction Engineering Division travel award*** 2014
from the American Institute of Chemical Engineers (AIChE)
- ***Kokes travel award*** from North American Catalysis Society 2013
- ***Full scholarship*** (all semesters) from Korea Research Foundation 2005-2009

TEACHING

Guest lecturer, UC Berkeley 2018

Course: Catalysis (undergraduate/graduate-level, CHEM ENG 245)

Responsibilities: Prepared and taught a lecture on the introduction of computational chemistry

Graduate Teaching Assistant, Northwestern University 2012-2014

Course: Molecular engineering and statistical mechanics (undergraduate/graduate-level, CBE 395)

Responsibilities: Held weekly office hours. Prepared and graded weekly assignments.

Guest lecturer, Northwestern University 2012

Course: Molecular engineering and statistical mechanics (undergraduate/graduate-level, CBE 395)

Responsibilities: Prepared and taught 1-hour lectures on the introduction of statistical mechanics and on Matlab

Graduate Teaching Assistant, Northwestern University 2011

Course: Chemical Engineering Laboratory (senior-level, CHEM_ENG 342)

Responsibilities: Prepared and taught operational procedures of experiments and data analyses.

STUDENTS MENTORED

- Mr. Ting Chun Lin, Iglesia Lab undergraduate researcher, UC Berkeley 2017-
- Mr. Neehar Duvvuri, Iglesia Lab undergraduate researcher, UC Berkeley 2018
- Mr. David Kuss, visiting master student from RWTH Aachen University, UC Berkeley 2017
- Mr. Maurice Vennwald, visiting master student from RWTH Aachen University, UC Berkeley 2017
- Ms. Izabela Samek, Snurr/Stair Lab Ph.D. student, Northwestern University 2015
- Ms. Rebecca Lu, Snurr Lab undergraduate researcher, Northwestern University 2014

SELECTED PRESENTATIONS

Oral Presentations

25th North American Meeting of the Catalysis Society Denver, CO, 2017

Title: Dioxygen activation routes in Mars-van Krevelen redox cycles on metal oxide catalysts

2016 AIChE Annual Meeting San Francisco, CA, 2016

Title: Dioxygen activation pathways in selective oxidations catalyzed by metal oxides

2016 Pacific Coast Catalysis Society Meeting Riverside, CA, 2016

Title: Mechanisms for reoxidation of reduced metal oxides by O₂: dioxygen activation pathways in Mars-van Krevelen catalytic cycles

2014 AIChE Annual Meeting

Atlanta, GA, **2014**

Title: Kinetic study of gas phase cyclohexene epoxidation over mesoporous TS-1 with H₂O₂ vapor

**Selected as a "best presentation" of the session*

Poster Presentations

24th North American Meeting of the Catalysis Society

Pittsburgh, PA, **2015**

Title: A kinetic study of vapor-phase cyclohexene epoxidation by H₂O₂ over mesoporous TS-1

23th North American Meeting of the Catalysis Society

Louisville, KY, **2013**

Title: Adsorption of CO₂ in photocatalysis

Catalysis Club of Chicago Spring Symposium

Naperville, IL, **2012**

Title: Adsorption of CO₂ in photocatalysis

MAJOR LEADERSHIP EXPERIENCE

Korean Students Association, Northwestern University

2011-2013

Role: President (2012-2013) and Vice President (2011-2012)

Responsibilities: Represented students in social events. Organized and ran student orientation, social events, and recruiting activities.

Class representative, Department of Chemical Engineering, Seoul National University 2007

Responsibilities: Organized student events and social activities.

REFERENCES

Professor Enrique Iglesia (Postdoc advisor),

Department of Chemical Engineering, UC Berkeley

iglesia@berkeley.edu

Professor Randall Snurr (Ph.D. advisor)

Department of Chemical and Biological Engineering, Northwestern University

snurr@northwestern.edu

Professor Peter Stair (Ph.D. advisor)

Department of Chemistry, Northwestern University

pstair@northwestern.edu

Dr. Stu Soled (Project collaborator)

Exxon Mobil

stu.soled@exxonmobil.com