Stephanie Kwon, Ph.D.
University of California at Berkeley
s-kwon@berkeley.edu
312.806.8611

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 *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 O_2 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 O_2 activation pathways using theoretical assessments based on DFT calculations. (*Manuscript in preparation for submission)*
- Elucidated HCOOH decomposition elementary steps on TiO_2 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 H_2O_2(g) on titanium silicate-1 (TS-1) catalysts by developing a flow reactor system that utilizes H_2O_2(g).
- Demonstrated propene oxidation with H_2O_2(g) to form acetone on Pd/Al_2O_3 and identified the reaction mechanisms via a detailed kinetic analysis, combined with DFT calculations
- Investigated the effects of basic oxide over-layers on TiO_2 catalysts for CO_2 adsorptions using DFT calculations and demonstrated the enhanced reactivities of MgO-decorated TiO_2 for CO_2 photo-reduction
- Identified O_2 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 $LaNiO_3$ 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 La_2O_3 during reactions.

PUBLICATION

1. **Kwon, S.**, P. Deshlahra, and E. Iglesia. (2019) Reactivity and Selectivity Descriptors of Dioxygen Activation Routes on Metal Oxides**,** *J. Cat., submitted*
2. **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.
3. **Kwon, S.**, P. Liao, P. C. Stair P. C, R. Q. Snurr (2016) Alkaline-earth metal-oxide overlayers on TiO_2: application toward CO_2 photoreduction, *Catal Sci Technol.,* 6, 7885–7895.
4. **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 H_2O_2 over mesoporous TS-1, *J. Cat.,* 323, 117-115.
5. 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.
6. 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**
Title: None-disclosure
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
Amount: Not available

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 O_2 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

- Ms. Sancialita Sathiyamoorthy, Iglesia Lab undergraduate researcher, UC Berkeley **2019**
- 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 Vennewald, 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

2018 AIChE Annual Meeting Pittsburgh, PA, **2018**

Title: Mechanistic Details of Formic Acid Dehydration on TiO_2 and ZrO_2 Catalysts

Title: Descriptors for Reactivity and Selectivity of Dioxygen Activation Routes on Metal Oxides

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 O_2: 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 H_2O_2 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 H_2O_2 over mesoporous TS-1

23th North American Meeting of the Catalysis Society Louisville, KY, **2013**

Title: Adsorption of CO_2 in photocatalysis

Catalysis Club of Chicago Spring Symposium Naperville, IL, **2012**

Title: Adsorption of CO_2 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