

# M. Alexander Ardagh, PhD

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## Education

### **Northwestern University**

PhD Chemical Engineering

Thesis: SiO<sub>2</sub> Deposition on Metal Oxides to Tune Acid Catalyst Behavior

Advisor: Justin Notestein

Committee Members: Linda Broadbelt, Peter Stair, and Neil Schweitzer

Evanston, IL

September 2018

### **University of Wisconsin**

BS Chemical Engineering; Graduation with Distinction

Research Advisor: James Dumesic

Madison, WI

August 2013

## Skills

**Programming Languages:** C, C++, Julia, Matlab, Python, R, SQL

**Molecular Modeling:** Avogadro, GAMESS, Gaussian, NWChem, Zacro, ZDOCK

**Cheminformatics:** DataWarrior, QSAR Toolbox

**Machine Learning:** Keras, R (caret), scikit-learn, Weka

**Spectroscopy:** FTIR, ICP-OES, <sup>1</sup>H, <sup>13</sup>C, <sup>27</sup>Al, <sup>29</sup>Si, and <sup>31</sup>P NMR, Raman, UV-Vis, XANES, XPS

**Quantification:** DSC, GC-FID, HPLC, MS, N<sub>2</sub> physisorption, Reaction kinetics, TGA, TPD, XRD

**Lab:** Homogeneous catalysis, Heterogeneous catalysis, Reactor construction, Sol-gel processing

## Research Experience

### **University of Minnesota**

Minneapolis, MN

**Postdoctoral Research Associate**, PI: Paul Dauenhauer

August 2018 – Present

- Demonstrated how dynamic catalyst operation in chemical reactors enhances the rate, conversion, and selectivity of chemical production such as ammonia for energy and methanol for chemicals
- Developed dynamic catalysis concept using C++, Julia, Matlab, and Python codes that automatically solve dynamic reactor equations and analyze the time-averaged chemical production
- Actively collaborated with University of Delaware and John Hopkins University postdocs and professors in the Catalysis Center for Energy Innovation (CCEI) to develop mathematical approach

### **Northwestern University**

Evanston, IL

**Graduate Research Assistant**, Advisor: Justin Notestein

January 2014 – July 2018

- Developed novel catalyst materials to efficiently and selectively convert bulky molecules (i.e. biomass, tar sands, waste oil) to useful chemicals and fuels such as jet fuel hydrocarbons and plastic
- Synthesized nanobowls catalysts using well controlled sol-gel processing of powder metal oxides. Used TEOS as an SiO<sub>x</sub> source, deposited SiO<sub>x</sub> layer-by-layer out of ethanol mixtures, and designed the nanobowls to match the size of the bulky raw materials using molecular templates
- Collaborated with students in Prof. Linda Broadbelt's group to combine computational and experimental studies of plastic production from citrus fruit peels (i.e. limonene epoxidation)
- Managed 10-15 graduate students and postdocs as the lab manager: directed lab cleanups, mediated disputes between lab members, and ensured access to Northwestern facilities and resources

## University of Wisconsin

Madison, WI

Undergraduate Research Assistant, Advisor: James Dumesic

September 2012 – August 2013

- Optimized xylose conversion and furfural production to provide research and development support for the startup company Glucan Biorenewables LLC
- Constructed flow reactors and tested both homogeneous and heterogeneous acid catalysts such as HCl, H<sub>2</sub>SO<sub>4</sub>, and mordenite for xylose conversion in flow reactors and glass vial batch reactors
- Obtained a maximum yield of 60% furfural using HCl at moderate temperatures ~120 °C. These results enabled scale up to pilot plant testing and further research and development has continued

## Leadership Experience

### Northwestern University

Evanston, IL

ChBE Teaching Committee

January 2016 – July 2018

- Directed teaching assistant peer mentoring program with 75-100 students over 5 quarters
- Revamped mentoring curriculum by introducing new topics and a roundtable discussion format
- Prepared presentations and delivered introductory seminars on teaching for 20-30 1st year ChBE graduate students to discuss teaching styles and common conflicts that TAs faced
- Led ChBE teaching committee of 10 members from May 2017 – July 2018; organized 3 programs including TA coffee chats with professors and created an annual TA handbook

### Northwestern University

Evanston, IL

Engineers for a Sustainable World

September 2015 – June 2016

- Planned and organized outreach events as ESW outreach co-chair with committee of 5 members to encourage community engagement between the public and Northwestern students
- Hosted urban sustainability event with 50-60 attendees and 6 speakers, including representatives of the Chicago Transportation Authority (CTA), Bike a Bee, and The Plant

## Selected Publications (4 of 15)

Shetty, M.; Ardagh, M. A.; Pang, Y.; Abdelrahman, O. A.; Dauenhauer, P. J. “Electric-Field Assisted Modulation of Surface Thermochemistry” in preparation for submission to *Nature Catalysis*

Ardagh, M. A.; Shetty, M.; Kuznetsov, A.; Zhang, Q.; Abdelrahman, O. A.; Vlachos, D. G.; Dauenhauer, P. J. “Catalytic Resonance Theory: Parallel Reaction and Pathway Control” *Chemical Science*, **2020**, *11*, 3501-3510

Ardagh, M. A.; Birol, T.; Zhang, Q.; Abdelrahman, O. A.; Dauenhauer, P. J. “Catalytic Resonance Theory: SuperVolcanoes, Catalytic Molecular Pumps, and Oscillatory Steady State.” *Catalysis Science & Technology*, **2019**, *9*, 5058-5076

**Cover Feature.** Ardagh, M. A.; Abdelrahman, O. A.; Dauenhauer, P. J. “Principles of Dynamic Heterogeneous Catalysis: Surface Resonance and Turnover Frequency Response.” *ACS Catalysis*, **2019**, *9* (8), 6929-6937

## Patents

Ardagh, M. A.; Frisbie, C. D.; Dauenhauer, P. J. “Dynamic Resonance of Heterogeneous Catalysis”. 2019, U.S. Provisional Patent, Application #62/812,146