

## DIANNE J. XIAO

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Department of Chemistry  
University of Washington  
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Seattle, WA 98195-1700

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### PROFESSIONAL EXPERIENCE

University of Washington

Assistant Professor, Department of Chemistry

2019–present

Stanford University

Postdoctoral Scholar (Advisor: Matthew W. Kanan)

2016–2019

Research focus: *CO<sub>2</sub> Insertion into C–H Bonds for Carboxylic Acid Synthesis*

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### EDUCATION

University of California, Berkeley

Ph.D. in Chemistry (Advisor: Jeffrey R. Long)

2016

Thesis: *Metal–Oxo and Dioxygen Chemistry in Metal–Organic Frameworks: Applications in Catalysis and Gas Separations*

Harvard University

A.B. *summa cum laude* in Chemistry (Advisor: Theodore Betley)

2011

Thesis: *Taming Manganese: Synthesis and Characterization of Trinuclear and Hexanuclear Manganese Clusters*

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### AWARDS AND HONORS

DOE Early Career Award

2021

ACS PRF Doctoral New Investigator Award

2020

GCEP and Precourt Student Energy Lecture Series, Distinguished Student Lecturer

2018

Arnold O. Beckman Postdoctoral Fellowship

2017–2019

Camille and Henry Dreyfus Postdoctoral Fellowship

2016–2017

National Science Foundation Graduate Research Fellowship

2012–2015

Outstanding Graduate Student Instructor Award

2012

Thomas T. Hoopes Thesis Prize

2011

Phi Beta Kappa

2010

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### SCIENTIFIC PUBLICATIONS

*At the University of Washington (underlined = undergraduate author, \* = corresponding author):*

- (23) Geary, J.; Wong, A. H.; **Xiao, D. J.**\* “Thermolabile cross-linkers for templating precise multicomponent metal–organic framework pores.” *J. Am. Chem. Soc.* **2021**, *143*, 10317–10323.
- (22) Do, M.; Rogers, D.; Kaminsky, W.; **Xiao, D. J.**\* “A robust synthetic route towards anisotropic metal–organic cages with tunable surface chemistry.” *Inorg. Chem.* **2021**, *60*, 7602–7606.

*Prior to the University of Washington:*

- (21) Reed, D. A.; **Xiao, D. J.**; Jiang, H. Z. H.; Chakarawet, K.; Oktawiec, J.; Long, J. R. “Biomimetic O<sub>2</sub> Adsorption in an Iron Metal–Organic Framework for Air Separation.” *Chem. Sci.* **2020**, *11*, 1698–1702.
- (20) **Xiao, D. J.**; Chant, E. D.; Frankhouser, A. D.; Chen, Y.; Yau, A.; Washton, N. M.; Kanan, M. W. “A Closed Cycle for Esterifying Aromatic Hydrocarbons with CO<sub>2</sub> and Alcohol.” *Nat. Chem.* **2019**, *11*, 940–947.

- (19) Reed, D. A.; Keitz, B. K.; Oktawiec, J.; Mason, J. A.; Runčevski, T.; **Xiao, D. J.**; Darago, L. E.; Crocellà, V.; Bordiga, S.; Long, J. R. "A Spin Transition Mechanism for Cooperative Adsorption in Metal–Organic Frameworks." *Nature* **2017**, *550*, 96–100.
- (18) Grosso-Giordano, N. A.; Yeh, A. J.; Okrut, A.; **Xiao, D. J.**; Grandjean, F.; Long, G. J.; Zones, S. I.; Katz, A. "Effect of Defect Site Preorganization on Fe(III) Grafting and Stability: A Comparative Study of Delaminated Zeolite vs Amorphous Silica Supports." *Chem. Mater.* **2017**, *29*, 6480–6492.
- (17) **Xiao, D. J.**; Oktawiec, J.; Milner, P. J.; Long, J. R. "Pore Environment Effects on Catalytic Cyclohexane Oxidation in Expanded Fe<sub>2</sub>(dobdc) Analogues." *J. Am. Chem. Soc.* **2016**, *138*, 14371–14379.
- (16) Zhang, W.; Kauer, M.; Halbherr, O.; Epp, K.; Guo, P.; Gonzalez, M. I.; **Xiao, D. J.**; Wiktor, C.; Xamena, L.; Francesc, X.; Woll, C.; Wang, Y.; Muhler, M.; Fischer, R. A. "Ruthenium Metal–Organic Frameworks with Different Defect Types: Influence on Porosity, Sorption, and Catalytic Properties." *Chem. Eur. J.* **2016**, *22*, 14297–14307.
- (15) Vogiatzis, K. D.; Haldoupis, E.; **Xiao, D. J.**; Long, J. R.; Siepmann, J. I.; Gagliardi, L. "Accelerated Computational Analysis of Metal–Organic Frameworks for Oxidation Catalysis." *J. Phys. Chem. C.* **2016**, *120*, 18707–18712.
- (14) Bloch, E. D.; Queen, W. L.; Hudson, M. R.; Mason, J. A.; **Xiao, D. J.**; Murray, L. J.; Flacau, R.; Brown, C. M.; Long, J. R. "Hydrogen Storage and Selective, Reversible O<sub>2</sub> Adsorption in a Metal–Organic Framework with Open Chromium(II) Sites." *Angew. Chem. Int. Ed.* **2016**, *55*, 8605–8609.
- (13) Mercado, R.; Vlasisavljevich, B.; Lin, L. –C.; Lee, K.; Lee, Y.; Mason, J. A.; **Xiao, D. J.**; Gonzalez, M.; Kapelewski, M. T.; Neaton, J. B.; Smit, B. "Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metal–Organic Frameworks." *J. Phys. Chem. C.* **2016**, *120*, 12590–12604.
- (12) Borycz, J.; Paier, J.; Verma, P.; Darago, L. E.; **Xiao, D. J.**; Truhlar, D. G.; Long, J. R.; Gagliardi, L. "Structural and Electronic Effects on the Properties of Fe<sub>2</sub>(dobdc) upon Oxidation with N<sub>2</sub>O." *Inorg. Chem.* **2016**, *55*, 4924–4934.
- (11) **Xiao, D. J.**; Gonzalez, M. I.; Darago, L. E.; Vogiatzis, K.; Gagliardi, L.; Long, J. R. "Selective, Tunable O<sub>2</sub> Binding in Cobalt(II)–Triazolate/Pyrazolate Metal–Organic Frameworks." *J. Am. Chem. Soc.* **2016**, *138*, 7161–7170.
- (10) Reed, D. A.; **Xiao, D. J.**; Gonzalez, M. I.; Darago, L. E.; Long, J. R. "Reversible CO Scavenging via Adsorbate-Dependent Spin State Transitions in an Iron(II)–Triazolate Metal–Organic Framework." *J. Am. Chem. Soc.* **2016**, *138*, 5594–5602.
- (9) Verma, P.; Vogiatzis, K.; Planas, N.; Borycz, J.; **Xiao, D. J.**; Long, J. R.; Gagliardi, L.; Truhlar, D. "Mechanism of Oxidation of Ethane to Ethanol at Iron(IV)–Oxo Sites in Magnesium-Diluted Fe<sub>2</sub>(dobdc)." *J. Am. Chem. Soc.* **2015**, *137*, 5770–5781.
- (8) Saeed, A.; Maya, F.; **Xiao, D. J.**; Najam-ul-Haqq, M.; Svec, F.; Britt, D. K. "Growth of a Highly Porous Coordination Polymer on a Macroporous Polymer Monolith Support for Enhanced Immobilized Metal Ion Affinity Chromatographic Enrichment of Phosphopeptides." *Adv. Funct. Mater.* **2014**, *24*, 5790–5797.
- (7) Kapelewski, M. T.; Geier, S. J.; Hudson, M. R.; Stück, D.; Mason, J. A.; Nelson, J. N.; **Xiao, D. J.**; Hulvey, Z.; Gilmour, E.; FitzGerald, S. A.; Head-Gordon, M.; Brown, C. M.; Long, J. R. "M<sub>2</sub>(m-dobdc) (M = Mg, Mn, Fe, Co, Ni) Metal–Organic Frameworks Exhibiting Increased Charge Density and Enhanced H<sub>2</sub> Binding at the Open Metal Site." *J. Am. Chem. Soc.* **2014**, *136*, 12119–12129.
- (6) **Xiao, D. J.**; Bloch, E. D.; Mason, J. A.; Queen, W. L.; Hudson, M.; Planas, N.; Borycz, J.; Dzubak, A. L.; Verma, P.; Lee, K.; Bonino, F.; Crocellà, V.; Yano, J.; Bordiga, S.; Truhlar, D. G.; Gagliardi, L.; Brown, C. M.; Long, J. R. "Oxidation of Ethane to Ethanol by N<sub>2</sub>O in a Metal–Organic Framework with Coordinatively Unsaturated Iron(II) Sites." *Nat. Chem.* **2014**, *6*, 590–595.
- (5) Zadrozny, J. M.; **Xiao, D. J.**; Long, J. R.; Atanasov, M.; Neese, F.; Grandjean, F.; Long, G. J. "Mössbauer Spectroscopy as a Probe of Magnetization Dynamics in the Linear Iron(I) and Iron(II) Complexes [Fe(C(SiMe<sub>3</sub>)<sub>3</sub>)<sub>2</sub>]<sup>1–0</sup>." *Inorg. Chem.* **2013**, *52*, 13123–13131.
- (4) Jeon, I. –R.; Park, J. G.; **Xiao, D. J.**; Harris, T. D. "An Azophenine Radical-Bridged Fe<sub>2</sub> Single-Molecule Magnet with Record Magnetic Exchange Coupling." *J. Am. Chem. Soc.* **2013**, *135*, 16845–16848.
- (3) Zadrozny, J. M.; **Xiao, D. J.**; Atanasov, M.; Long, G. J.; Grandjean, F.; Neese, F.; Long, J. R. "Magnetic blocking in a linear iron(I) complex." *Nat. Chem.* **2013**, *5*, 577–581.
- (2) Fout, A. R.; **Xiao, D. J.**; Zhao, Q.; Harris, D. T.; King, E. R.; Eames, E. V.; Zheng, S. –L.; Betley, T. A. "Trigonal Mn<sub>3</sub> and Co<sub>3</sub> Clusters Supported by Weak-Field Ligands: A Structural, Spectroscopic,

Magnetic, and Computational Investigation into the Correlation of Molecular and Electronic Structure.” *Inorg. Chem.* **2012**, *51*, 10290-10299.

- (1) Fout, A. R.; Zhao, Q.; **Xiao, D. J.**; Betley, T. A. “Oxidative Atom-Transfer to a Trimanganese Complex To Form  $Mn_6(\mu^6-E)$  ( $E = O, N$ ) Clusters Featuring Interstitial Oxide and Nitride Functionalities.” *J. Am. Chem. Soc.* **2011**, *133*, 16750-16753.
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#### PATENTS

Long, J. R.; Xiao, D. J. “Redox-Active Metal-Organic Frameworks for the Catalytic Oxidation of Hydrocarbons.” US10058855B2, 2018.

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#### SELECTED INVITED PRESENTATIONS

*At the University of Washington:*

University of Washington Molecular Engineering Materials Center **2020**

*Prior to the University of Washington:*

Future Faculty in Chemistry Symposium, Department of Chemistry and Chemical Biology, **2018**  
Harvard University, Cambridge, MA

249<sup>th</sup> ACS National Meeting, Denver, CO **2015**

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#### SELECTED CONTRIBUTED PRESENTATIONS

*At the University of Washington:*

ACS Spring 2021 (virtual meeting) **2021**

*Prior to the University of Washington:*

257<sup>th</sup> ACS National Meeting, Orlando, FL **2019**

Inorganic Chemistry Gordon Research Conference, Biddeford, ME **2018**

255<sup>th</sup> ACS National Meeting, New Orleans, LA **2018**

Inorganic Chemistry Gordon Research Conference, Biddeford, ME **2016**

250<sup>th</sup> ACS National Meeting, Boston, MA **2015**

248<sup>th</sup> ACS National Meeting, San Francisco, CA **2014**

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#### TEACHING EXPERIENCE

*At the University of Washington:*

Chem 165: Honors General Chemistry **2020–present**

Median course evaluations: SP21 4.8/5.0, SP20 4.4/5.0

Chem 312: Inorganic Chemistry **2019–present**

Median course evaluations: AU20 4.3/5.0, AU19 3.7/5.0

*Before the University of Washington:*

Graduate Student Instructor, Chem 104B: Advanced Inorganic Chemistry, UC Berkeley **2013, 2014**

Graduate Student Instructor, Chem 4A: General Chemistry, UC Berkeley **2011**

*Received Outstanding Graduate Student Instructor award*

Laboratory Teaching Fellow, Chem S-20: Organic Chemistry, Harvard University **2010**

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#### OUTREACH ACTIVITIES

Burke Museum Girls in Science Program (*planned*) **2021–present**

Guest speaker, Shorewood High School AP Environmental Science **2021**

Mentor, the Chemistry Women Mentorship Network (Chem WMN) **2019–present**

