Dianne J. Xiao

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Department of Chemistry
University of Washington
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Professional Experience

University of Washington
Assistant Professor, Department of Chemistry — **2019**

Stanford University
Postdoctoral Scholar (Advisor: Matthew W. Kanan) — **2016–2019**
Research focus: *CO_2 Insertion into C–H Bonds for Carboxylic Acid Synthesis*

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*

Awards and Honors

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**
Harvard College Research Program Award	**2010**
Harvard Detur Book Prize	**2008**
Harvard Program for Research in Science and Engineering Fellowship	**2008**

(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_2 and Alcohol." *Nat. Chem.* **2019**, accepted.

(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_2(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_2 Adsorption in a Metal–Organic Framework with Open Chromium(II) Sites." *Angew. Chem. Int. Ed.* **2016**, 55, 8605–8609.

(13) Mercado, R.; Vlaisavljevich, 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_2(dobdc) upon Oxidation with N_2O." *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_2 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_2(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_2(*m*-dobdc) (M = Mg, Mn, Fe,

Co, Ni) Metal–Organic Frameworks Exhibiting Increased Charge Density and Enhanced H_2 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_2O 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 $[Fe(C(SiMe_3)_3)_2]^{1-/0}$." *Inorg. Chem.* **2013**, *52*, 13123-13131.

(4) Jeon, I. –R.; Park, J. G.; **Xiao, D. J.**; Harris, T. D. "An Azophenine Radical-Bridged Fe_2 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_3 and Co_3 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 $Mn_6(\mu^6\text{-E})$ (E = O, N) Clusters Featuring Interstitial Oxide and Nitride Functionalities." *J. Am. Chem. Soc.* **2011**, *133*, 16750-16753.

Patents

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

Invited Presentations

"Hydrocarbon Functionalization in Porous Materials" – Future Faculty in Chemistry Symposium, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA **2018**

Selected Contributed Presentations

"C–H Carboxylation of Aromatic Hydrocarbons using CO_2" – Poster at Inorganic Chemistry Gordon Research Conference, Biddeford, ME **2018**

"Carbonate-Promoted C–H Carboxylation of Aromatic Hydrocarbons with CO_2" – 255th ACS National Meeting, New Orleans, LA **2018**

"Hydrocarbon Oxidations in Iron Metal–Organic Frameworks" – Poster at Inorganic Chemistry Gordon Research Conference, Biddeford, ME **2016**

"Dioxygen Activation in a Cobalt Metal-Organic Framework for O_2/N_2 separations and catalysis" – 250th ACS National Meeting, Boston, MA **2015**

"Hydrocarbon Oxidations Using Iron Metal-Organic Frameworks" – 248th ACS National Meeting, San Francisco, CA **2014**

Teaching Experience

Graduate Student Instructor, Chem 104B, Advanced Inorganic Chemistry, UC Berkeley **2013, 2014**
Graduate Student Instructor, Chem 4A, General Chemistry and Quantitative Analysis, UC Berkeley **2011**
Laboratory Teaching Fellow, Chem S-20, Organic Chemistry (summer course), Harvard University **2010**