Jiayi Xu

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EDUCATION

Ph.D. candidate, Chemical Engineering, Kansas State University 02/2021
B.S. Chemical Engineering; Secondary major, Biological Engineering, Kansas State University 05/2016

RESEARCH EXPERIENCE

Chemical Sciences and Engineering Division, Argonne National Lab

Postdoctoral Appointee under Dr. Cong Liu **02/2021 - Present**

- Electronic cooperativity in supported single sites for catalytic C-C and C-H bonds functionalization
- Computational studies on lithium ion batteries.

Department of Chemical Engineering, Kansas State University

Graduate Research Assistant under Dr. Bin Liu **08/2016 - 02/2021**

Dissertation: "Design Functional Catalytic Materials from First-Principles Methods for Methanol Fuel Cells"

- Investigation of oxygen reduction reaction (ORR) and methanol oxidation reaction (MOR) over Pt supported by vertically aligned carbon nanofibers
- Design of Platinum group metal free catalyst for ORR
- Molecular modeling of C1 conversion to value-added chemicals via heterogeneous catalysis

Undergraduate Research Assistant under Dr. Keith Hohn and Dr. Bin Liu **05/2013 - 05/2016**

- Investigation of confinement effect of Cu loaded zeolite towards dehydration of 2,3-butanediol
- Investigation of acidity distribution of mesoporous silica catalyst via single molecule spectroscopy
- Investigation of the influence of basicity and acidity on dehydration of 2,3-butanediol

AWARDS

- 17th International Congress on Catalysis travel award, $500 03/13/2020
- 2nd Great Plain Catalysis Symposium travel award, $150 04/12/2019
- William H. & Virginia Honstead Fellowship Scholarship, $500 03/11/2019
- Engineering Research and Graduate Program (ERGP) Funding, $500 11/14/2018
- Sustainable Energy Award, $1060 10/24/2018
- Graduate Student Council (GSC) Travel Award, $400 10/22/2018
- Chemical Engineering Excel, $1800 05/2017
- Undergraduate Research Poster Forum, 3rd Place, $100 12/2014
- Engineering Scholarships, $2000 10/2013

PUBLICATIONS

1. **Xu. J.**; Elongovan. A.; Li, J.; Liu, B. Stabilization and Catalytic Influence of Multi-edge Carbon Support on Pt ORR Catalysts. (in preparation)

2. Radaha, E. A.; Vlies, A. J. D.; **Xu**, **J.**; Liu, B.; Hasegawa, U. Reactive Oxygen Species Sensitive Polymeric Micelles for Anti-Cancer Drug Delivery. (**Submitted to *ACS Appl. Mater. Interfaces***)

3. **Xu**. **J.**; Elongovan. A.; Li, J.; Liu, B. Dual Metal Sites Embedded in Graphene for Oxygen Reduction Reaction: A theoretical Study. ***J. Phys. Chem. C***, 2021, 125, 4, 2334-2344.

4. Elangovan, A.; **Xu, J.**; Sekar, A.; Liu, B.; Li, J. CO Tolerant Platinum-Based Catalysts on a Nitrogen-Doped 3D Graphitic Carbon Support for Methanol Oxidation. ***ChemcatChem***, 2020, 12, 1-14

5. Elangovan, A.; **Xu**, **J.**; Pandey, G.; Brown, E.; Liu, B.; Li, J. Vertically Aligned Carbon Nanofiber Array with Conically Stacked Graphitic Structure as an Efficient Three-dimensional Catalyst Support to Enable

Ultralow Pt Loadings for Oxygen Reduction Reactions, ***J. Electro. Soc.*** **2020** 167 (6), 066523

6. **Xu**, **J.**; Liu, B. Intrinsic Properties of Nitrogen-Rich Carbon Nitride for Oxygen Reduction Reaction, ***Appl. Surf. Sci.*** **2019** 500, 144020.
7. Xie, J.; **Xu**, **J.**; Sun, X.; Higgins, D. A.; Hohn, K. L. Exploring Microenvironment Acidity Inside the solvent-Filled Pores of Mesoporous Silica Thin Filems via Single-Molecule Spectroscopy, ***J. Phys. Chem. C*** **2019**, 123 (33), 20333-20341.

8. Wang, L.; Zhang, Y.; **Xu**, **J.**; Diao, W.; Karakalos, S.; Liu, B.; Song, X.; Wu, W.; He, T.; Ding, D. Non-oxidative Dehydrogenation of Ethane to Ethylene over ZSM-5 Zeolite Supported Iron Catalysts, ***Appl. Catal. B: Environ.*** **2019** 256, 117816.

9. **Xu, J.**; and Liu, B. Modeling C-H bond Activation and Oxidation of C1-C3 Alkanes over Cu-MOR using First-Principles Method, ***J. Phys. Chem. C*** **2019** 123, 10356-10366.

10. Oh, S. **Xu, J.**; Tran, D.; Liu, B.; Liu, D. Effects of Controlled Crystalline Surface of Hydroxyapatite on Methane Oxidation Reactions, ***ACS Catal.*** **2018** 8 (5), 4493-4507.

11. Zheng, Q.; **Xu**, **J.**; Liu, B.; Hohn, K. L. Mechanistic Study of the Catalytic Conversion of 2,3-Butanediol to Butenes, ***J. Catal***. **2018** 360, 221-239.

12. Zheng, Q.; Grossardt, J.; Almkhelfe, H.; **Xu**, **J.;** Grady, B. P.; Douglas, J. T.; Amama, P. B.; Hohn, K. L. Study of Mesoporous Catalysts for Conversion of 2, 3-butanediol to Butenes, ***J. Catal.*** **2017** 354, 182-196.

13. Zeng, F.; Tenn, W. J.; Aki, S. N.; **Xu, J.**; Liu, B.; Hohn, K. L. Influence of Basicity on 1, 3-butadiene Formation from Catalytic 2, 3-butanediol Dehydration over γ-alumina, ***J. Catal.*** **2016** 344, 77-89.

14. Sun, X.; Xie, J.; **Xu, J.**; Higgins. H. D.; Hohn, H. L. Single-Molecule Studies of Acidity Distributions in Mesoporous Aluminosilicate Thin Films, ***Langmuir*** **2015** 31 (20), 5667-5675.

CONFERENCE PRESENTATIONS

- **Xu, J.** and Liu, B. Noble-Metal Free Oxygen Reduction Electrocatalysts Based on Graphitic Carbon Nitride, **Virtual AIChE Annual Meeting**, Nov. 16th-20th, 2020 (Poster)

- **Xu, J.** and Liu, B. Catalyst Design for Oxygen Reduction Reaction Using Molecular Modeling, **Virtual AIChE Annual Meeting**, Nov. 16th-20th, 2020 (Poster)

- **Xu, J.** and Liu, B. Design of Atomically Dispersed, Non-Precious Catalyst for Oxygen Reduction Reaction, **Tim Taylor Department of Chemical Engineering, Kansas State University,** Manhattan, KS**,** May, 19th, 2020 (Invited Talk)

- **Xu, J.**; Elangovan, A.; Li, J.; and Liu, B. Molecular level understanding of Cyclic voltammetry for methanol oxidation over Pt-based catalysts, **NAM26**, Chicago, IL, Jun. 25th, 2019 (Poster)

- **Xu, J.**; and Liu, B. Oxygen reduction reaction over Pt-supoorted vertically aligned carbon nanofiber, **Great Plains Catalysis Society**, Bartlesville, OK, USA, Apr, 12th, 2019 (Oral)

- **Xu, J.**; Elangovan, A.; Li, J.; and Liu, B. Oxygen reduction reaction over a novel 3D Pt-supported vertically aligned carbon nanofiber, **AIChE Annual Meeting**, Pittsburgh, PA, USA, Oct. 27th to Nov. 2nd, 2018. (Oral)

- **Xu, J.**; Zheng, Q.; Hohn, KL; and Liu, B. Understanding catalytic bifunctionality of Cu/ZSM5 and Cu/Y

zeolites for biomass conversions, **Great Plains Catalysis Society**, Manhattan, KS, USA, Apr. 18th, 2018. (Poster)

- **Xu, J.**; Xie, J.; Sun, X.; Higgins, D.; and Hohn, KL. Investigation acidity inside pores of SBA 15 via single molecule spectroscopy, **ACS Midwest Regional Meeting**, Lawrence, KS, USA, Oct. 18th-20th, 2017. (Oral)

- **Xu, J.** and Liu, B. Cu-oxo complexes supported in MOR zeolites as active sites for methane-to-methanol conversion, **ACS Midwest Regional Meeting**, Lawrence, KS, USA, Oct. 18th-20th, 2017. (Oral)

- **Xu, J.**; Zheng, Q.; Hohn, KL. and Liu, B. Understanding catalytic bifunctionality of Cu/ZSM5 and Cu/Y zeolites for biomass conversions, **ACS Midwest Regional Meeting**, Lawrence, KS, USA, Oct. 18th-20th, 2017. (Poster)

ACTIVITIES

- Reviewer for Materials Today Energy, International Journal of Quantum Chemistry, ChemistrySelect.

TEACHING EXPERIENCE

Department of Chemical Engineering, Kansas State University

- Teaching assistant for CHE 561 Chemical Process Dynamics Control — Spring 2020
- Teaching assistant for CHE 802, Top. Molecular Modelling — Fall 2019
- Teaching assistant for CHE 320, Chemical Process Analysis — Spring 2017
- Teaching assistant for CHE 550, Chemical Reaction Engineering — Fall 2016

SKILLS

- Software: VASP, LAMMPS, NWCHEM, Gaussian, GAMESS, Mathematica, Polymath, AspenPlus, Microsoft Office
- Programming language: Python, Fortran, Wolfram