Shuting Xiang

Department of Materials Science and Chemical Engineering, Stony Brook University.
shuting.xiang@stonybrook.edu | (573) 999-0074 | pronouns: she/her

EDUCATION

Ph.D. in Materials Science, Stony Brook University**,** Stony Brook, NY — Expected May 2025
M.S. in Chemical Engineering, Columbia University, New York, NY — Aug. 2017 – Feb. 2019
B.S. in Chemical Engineering, University of Missouri, Columbia, MO — Aug. 2014 – Dec. 2016
B.S. in Chemical Engineering, Wuhan Institute of Technology, China — Aug. 2012– Jun. 2014
(Joint Undergraduate Chemical Engineering Program of MU and WIT)

EXPERTISE

As part of my PhD research, I developed methods of materials characterization based on advanced applications of X-ray absorption spectroscopy. I combined XAS with complementary techniques for studies of catalytic systems with controlled degree of nuclearity. Those ranged from "single atoms", clusters, and nanoparticles to bulk mono- and multimetallic alloy materials. I demonstrated that unique new functionalities can be rationally designed after the atomistic details of reactions and processes are understood. I am keen to extend my methods to other materials and processes.

RESEARCH EXPERIENCE

Stony Brook University & Brookhaven National Laboratory — Jan. 2020 – Present
Ph.D. Student, advisor: Prof. Anatoly Frenkel

New Catalytic Pathways for CO and CO_2 Conversions

- Leading a project on CO oxidation on Co "single-atom" catalysts on C_3N_4. Comparison of the roles of active sites in thermal and photo-catalysis. Mentoring a new Ph.D. student in the group.
- Led a project on CO_2 hydrogenation on Rh-based catalysts within a manganese oxide framework and investigated their performance and structure via DRIFTS, TPR, XAFS, XRD, and TEM-EDS. Published (1st author): *Appl. Catal. A: General*.
- Developed new methods for machine learning – assisted structural characterization of XAFS, to understand the reaction mechanism at atomic level. Published (1st author): *PCCP*.
- Expert knowledge of XAFS operando experiments, data analysis, and reaction setup.

Mechanism of Ethanol Dehydrogenation over Dual-Atom Pairs in Trimetallic Alloys

- Leading on X-ray absorption study (data analysis, modeling, and interpretation), and manuscript preparation for the research on the role of Pt-Cr pair for enhanced ethanol dehydrogenation activity in AgPtCr alloy.
- Leading the coordination of efforts of PIs and their group members from SBU, UF, BNL, and Tulane University.

Collaborative Projects Using my Expertise in Catalysis and XAFS methods

- Conducted X-ray absorption near edge structure (XANES) analysis and extended X-ray absorption fine structure (EXAFS) simulation of multiple catalytic systems ranging from supported ReO_x catalysts for Olefin metathesis, to iron porphyrin used in oxygen reduction, to Cu@TiOx Core@Shell Catalyst for CO_2 hydrogenation, among others.

Columbia University & Brookhaven National Laboratory
Officer of Research, advisor: Prof. Oleg Gang — Feb. 2019 – Dec. 2019

Biosensor on Etched Silicon Substrate

- Led a project on the development of a platform for optical sensing of DNA and antibodies using specifically designed nanoscale surfaces.
- Investigated the biosensor on etched silicon surface to detect target DNA sequences and human IgG and explored its sensitivity and selectivity.
- Fabricated regular, uniform patterns from block copolymer thin films through microphase separation on silicon substrate and investigated the infiltration of the pattern with inorganic material using sequential, self-limiting exposures to gaseous precursors.

- Explored and measured the anti-reflection of the etched silicon substrate patterned by block copolymer.

Columbia University
M.S. Student, advisor: Prof. Oleg Gang Jan. 2018 – Jan. 2019
Lattice Engineering through DNA Origami Framework
- Synthesized scaffolded and self-assembled the DNA origami frames into open three-dimensional frameworks to form lattice of different structures based on the prescribed binding modalities and characterized the 3D lattice with small-angle X-ray scattering (SAXS).
- Explored the loading of 3D DNA origami frame lattices with various functional nanomaterials (i.e. metallic nanoparticles, enzymes, etc.).
- Functionalized gold nanoparticles with a target number of DNA sequences per particle and improved the yield of DNA origami and nanoparticle conjugates depending on their valency.

University of Missouri
Undergraduate Research Assistant, advisor: Prof. Maria Fidalgo Sep. 2015 – Aug. 2017
Nanomaterials for Water Treatment Process
- Synthesized various novel materials for water treatment process, including molecularly imprinted porous films (MIPs) for the capture of testosterone, zwitterionic polymer coated ceramic nanomaterials for natural organic matter adsorption, two-dimension Fe_3O_4 nanosheet for arsenic adsorption.
- Investigated the performance of these materials for water treatment process, such as the saturation level, adsorption ability, fouling resistance, selectivity, and recyclability.
- Characterized adsorbent properties with SEM, TEM, XRD, BET, and DLS.

PUBLICATIONS

1. Z. Li, X. Li, R. Wang, S. Roy, C. S. Gerke, **S. Xiang**, M. A. C. Mata, A. Mathur, L. Zhang, D.-Z. Lin, T. Li, K. N. Jayarapu, A. Liu, L. Gupta, A. I. Frenkel, V. S. Thoi, P. M. Ajayan, Y. Liu. Electro-activated indigos intensify ampere-level CO_2 reduction to CO on silver catalysts. (submitted 10, 2024) *Nature Catalysis*
2. Z. Li, P. Wang, G. Han, S. Yang, S. Roy, **S. Xiang**, J. D. Jimenez, V. K. R. Kondapalli, X. Lyu, J. Li, A. Serov, R. Li, V. Shanov, S. D. Senanayake, A. I. Frenkel, P. M. Ajayan, Y. Sun, T. P. Sentfle, J. Wu. Ampere-level co-electrosynthtesis of formate from CO_2 reduction paired with formaldehyde dehydrogenation reactions. (submitted 09, 2024) *Nature Communications*
3. J. S. Kahn, B. Minevich, A. Michelson, H. Emamy, K. Kisslinger, **S. Xiang**, S. K Kumar, J. Wu, A. Yun, H. Ji, N. Yu, O. Gang. Encoding Hierarchical 3D Architecture through Inverse Design of Programmable Bonds. (submitted 07, 2024) *Nature Materials.*
4. **S. Xiang**, J. D. Jimenez, L. F. Posada, S. J. B. Rubio, H. S. Khanna, S. Hwang, D. Leshchev, S. L. Suib, A. I. Frenkel, and S. D. Senanayake. CO_2 Hydrogenation over Rhodium Cluster Catalyst Nucleated within Secondary Ion Stabilized Manganese Oxide Framework. *Applied Catalysis A, General,* **2024**, 683, 119845.
5. K. Deng, X. Chen, J. Moncada, K. L. Salvatorel, N. Rui, W. Xu, **S. Xiang**, N. Marinkovic, A. I. Frenkel, G. Zhou, S. S. Wong, J. A. Rodriguez. Observing Chemical and Morphological Changes in a Cu@TiOx Core@Shell Catalyst: Impact of Reversible Metal-Oxide Interactions on CO_2 Activation and Hydrogenation. *ACS Catalysis,* **2024**, 14, 11832-11844.
6. T. Han, Y. Li, T. Wu, D. M. Meira, **S. Xiang**, Y. Cao, I. Lee, X. Zhou, D. Jiang, A. I. Frenkel, F. Zaera1. Remote Activation of H–H Bonds by Platinum in Dilute Alloy Catalysts. *ACS Catalysis,* **2024**, 14, 7157-7165.
7. A. Michelson, A. Subramian, K. Kisslinger, N. Tiwale, **S. Xiang**, E. Shen, H. Yan, C.-Y. Nam, O. Gang. Three-dimensional Nanoscale Metal, Metal Oxide, and Semiconductor Frameworks through DNA-programmable Assembly and Templating. *Science Advances,* **2024**, 10(2), eadl0604.
8. Z. Li, P. Wang, X. Lyu, V. K. R. Kondapalli, **S. Xiang**, J. D. Jimenez, L. Ma, T. Ito, T. Zhang, J. Raj, Y. Fang, Y. Bai, J. Li, A. Serov, V. Shanov, A. I. Frenkel, S. D. Senanayake, S. Yang, T.

P. Senftle and J. Wu. Directing CO_2 electroreduction pathways for selective C_2 product formation using single-site doped copper catalysts. *Nature Chemical Engineering,* **2024**, 1, 159-169.

9. Z. An, P. Yang, D. Duan, J. Li, T. Wan, Y. Kong, S. Caratzoulas, **S. Xiang**, J. Liu, L. Huang, A. I. Frenkel, Y.-Y. Jiang, R. Long, Z. Li, D. Vlachos. Highly Active, Ultra-Low Loading Single-Atom Iron Catalysts for Catalytic Transfer Hydrogenation. *Nature Communications*, **2024**, 14, 6666.

10. J. Li, P. Huang, F. Guo, J. Huang, **S. Xiang**, K. Yang, N. A. Deskins, V. S. Batista, G. Li, A. I. Frenkel. X-ray Absorption Spectroscopy Studies of a Molecular CO_2-Reduction Catalyst Deposited on Graphitic Carbon Nitride. *The Journal of Physical Chemistry,* **2023**, 127, 3626-3633.

11. L. Asor, J. Liu, **S. Xiang**, N. Tessler, A.I. Frenkel, U. Banin. Zn-doped P-type InAs Nanocrystal Quantum Dots. *Advanced Materials,* **2022**, 35, 220832.

12. B. Zhang, **S. Xiang**, A. I. Frenkel, I. Wachs. Molecular Design of Supported MoO_x Catalysts with Surface TaO_x Promotion for Olefin Metathesis. *ACS Catalysis,* **2022**, 12, 3226-3237.

13. **S. Xiang**, P. Huang, J. Li, Y. Liu, N. Marcella, P. K. Routh, G. Li, and A. I. Frenkel. Solving the Structure of "Single-atom" Catalysts Using Machine Learning-Assisted XANES Analysis. *Physical Chemistry Chemical Physics,* **2022**, 24, 5116-5124.

14. Q. Hua, K. E. Madsen, A. M. Esposito, X. Chen, T. J. Woods, R. T. Haasch, **S. Xiang**, A. I. Frenkel, T. T. Fister, and A. A. Gewirth. Effect of Support on Oxygen Reduction Reaction Activity of Supported Iron Porphyrins. *ACS Catalysis,* **2021**, 12, 1139-1149.

15. A. Michelson, H. Zhang, **S. Xiang**, O. Gang. Engineering Silicon Carbide Three-Dimensional Frameworks through DNA-Prescribed Assembly. *Nanoletter,* **2021**, 21(4), 1863-1870.

16. B. Zhang, S. Lwin, **S. Xiang**, A. I. Frenkel, I. E. Wachs. Tuning the Number of Active Sites and Turnover Frequencies by Surface Modification of Supported $ReO_4/(SiO_2Al_2O_3)$ Catalysts for Olefin Metathesis. *ACS Catalysis,* **2021**, 11, 2412-2421.

17. Z. Lin, H. Emamy, B. Minevich, Y. Xiong, **S. Xiang**, S. K. Kumar, Y. Ke, O. Gang. Engineering Organization of DNA Nano-Chambers through Dimensionally Controlled and Multi-Sequence Encoded Differentiated Bonds. *Journal of the American Chemical Society,* **2020**, 142(41), 17531-17542. **(Cover)**

18. M. Storms, A. J. Kadhem, **S. Xiang**, M. Bernards, G. J. Gentile and M. Fidalgo de Cortalezzi. Enhancement of Fouling Resistance of Zwitterion Coated Ceramic. *Membranes,* **2020**, 10(9), 210.

19. Y. Xiong, S. Yang, Y. Tian, A. N. Michelson, **S. Xiang**, H. Xin and O. Gang. Three-Dimensional Patterning of Nanoparticles by Molecular Stamping. *ACS Nano,* **2020**, 14(6), 6823-6833.

20. Z. Lin, Y. Xiong, **S. Xiang** and O. Gang. Controllable Covalent-bound Nanoarchitectures from DNA Frames. *Journal of the American Chemical Society,* **2019**, 141(17), 6797-6801.

21. A. Kadhem, **S. Xiang**, S. Nagel, C.-H. Lin, M. Fidalgo de Cortalezzi. Photonic Molecularly Imprinted Polymer Film for Detection of Testosterone in Aqueous Samples. *Polymers,* **2018**, 10(4), 349.

22. H. Luo, F. Cheng, W. Hu, J. Wang, **S. Xiang**, M. Fidalgo de Cortalezzi. 2D Fe_3O_4 Nanosheet for effective Arsenic Removal. *Journal of Contemporary Water Research and Education,* **2017** 160 (1), 132-143.

MANUSCRIPTS IN PREPARATION

- **S. Xiang**, A. John, Q. Qian, A. Deskins, G. Li, A. I. Frenkel. Utilization of Dynamic Time Warping on Similarity Calculation of XANES Spectra.
- **S. Xiang**, M. Knecht, A. I. Frenkel. Review on Machine Learning-XAFS studies on Bimetallic Nanoparticles in Catalysis.
- Q. Li, S. Cheong, **S. Xiang**, A. I. Frenkel, Y. Yang, N. M. Bedford, I. Onishi, A. R. Poerwoprajitno, Z. R. Ramadhan, W. Schuhmann, J. J. Gooding, R. D. Tilley. Platinum Atomic Strings and Clusters on Ruthenium Hourglass Nanoparticles for Enhanced Hydrogen Evolution Reaction.

- J. F. Weaver, **S. Xiang**, J. Jamir, U. Kust, L. Ramisch, A. Grespi, H. Wallander, J. Zerterberg, S. Arias, E. Fornero, P. K. Routh, S. Zhang, A. Boscoboinik, M. M. Montemore, C. H. Sykes, J. Knudsen, J. Biener, L. Merte, A. I. Frenkel, Selective catalysis promoted by dual-atom pairing in trimetallic alloys: Ethanol dehydrogenation over PtCrAg films.

PATENT

1. O. Gang, B. Minevich, H. Emamy, **S. Xiang**, J. S Kahn, A. Michelson, K. Kisslinger, S. Kumar. Encoding an Assembly of Three-Dimensional Hierarchically Organized Nanoparticle Architectures through Chromatic Bonds. Application number: 18217812. **01, 11, 2024**

AWARD

CATL-ChemCatBio Graduate Student Travel Award — Fall 2024 ACS

CONFERENCE PRESENTATION

- ACS Fall 2024, talk — Denver, CO, USA; Aug. 2024
- NSLS-II & CFN User's Meeting, poster — Upton, NY, USA; May 2024
- MSCE Research Day, talk and poster — Stony Brook, NY, USA; Nov. 2023
- ACS Fall 2023, talk — San Francisco, CA USA; Aug. 2023
- NAM28, talk — Providence, RI, USA; Jun. 2023
- 2022 Annual AIChE Meeting, talk — Phoenix, AZ, USA; Nov. 2022

LEADERSHIP & SERVICE

Instructor

- Synchrotron Catalysis Consortium (SCC) Short Course at BNL — Nov. 2022-2024

Volunteer

- Summer Sunday at Center for Functional Nanomaterials at BNL — July 2019
- Columbia Chemical Engineering Fuel Cell Car Demonstration and Competition — Sep. 2017

Ambassador — Sep. 2017– Feb. 2019

- Master of Science Program Ambassador for Department of Chemical Engineering in Columbia University in the City of New York

SKILLS

- Software – Expert level of Python, in addition to the common data processing and analysis packages, including XANES and EXAFS.
- Techniques – Single Particle Tracking, X-Ray Diffraction (XRD), X-Ray Photoelectron Spectroscopy (XPS), Ultraviolet-visible Spectroscopy (UV-Vis), High-performance Liquid Chromatography (HPLC), Atomic Absorption Spectroscopy (AAS), Fourier-transform Infrared Spectroscopy (FT-IR), Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), Contact Angle Measurement and Small Angle X-ray Scattering (SAXS), Atomic Layer Deposition (ALD), Sequential Infiltration Synthesis (SIS), Atomic Force Microscope (AFM), X-ray Absorption Fine Structure (XAFS) Analysis, Linear Combination Fitting (LCF), Principal Component Analysis (PCA), Artificial Neural Network (ANN), K-means clustering, Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS), NMR, temperature programmed reaction (TPR).

REFERENCES

- Prof. Anatoly Frenkel — Department of Materials Science and Chemical Engineering, Stony Brook University, Stony Brook, NY 11794, anatoly.frenkel@stonybrook.edu
- Prof. Oleg Gang — Department of Chemical Engineering, Columbia University, New York, NY, 11027, og2226@columbia.edu

- Dr. Sanjaya D. Senanayake
  Chemistry Division
  Brookhaven National Laboratory, Upton, NY 11973
  ssenanay@bnl.gov
- Prof. Gonghu Li
  College of Engineering and Physical Sciences
  University of New Hampshire, Durham, NH 03824
  gonghu.Li@unh.edu
- Prof. Jose Rodriguez
  Chemistry Division
  Brookhaven National Laboratory, Upton, NY 11973
  rodrigez@bnl.gov