

**Xiaoyu Wang**

Postdoctoral Fellow  
Department of Chemical and Biomolecular Engineering  
University of Notre Dame  
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**EDUCATION**

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**Bachelor of Science: Applied Chemistry** 2008—2012

Sichuan University, Chengdu, Sichuan Province, China

**Master of Engineering: Chemical Engineering** 2013—2015

Illinois Institute of Technology, Chicago, IL, U.S.

**Doctor of Philosophy: Chemical Engineering** 2015—2020

Illinois Institute of Technology, Chicago, IL, U.S.

PhD Dissertation Title: “Using Computational Molecular Modeling to Study Transport Processes of Interest in Separations”

Dissertation Advisor: Dr. Sohail Murad; Dr. Cynthia J. Jameson

**RESEARCH EXPERIENCE**

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**Postdoctoral Research Associate** 05/2020 - Present

University of Notre Dame, Notre Dame, IN, U.S.

Role: To develop and utilize molecular dynamics simulations to understand how additives affect the thermophysical properties of deep eutectic solvents and to use simulations to understand how templating agents affect the performance of zeolite catalysts.

**Graduate Research Assistant** 05/2015 - 05/2020

Illinois Institute of Technology, Chicago, IL, U.S.

Role: To investigate chiral drug separation processes on polysaccharide-based polymer surfaces; to study fluid separations through zeolite membranes and provide insights when separations fail; to use molecular dynamics simulations to characterize the anisotropy of thermal conductivity at interfaces.

**NSF Funded Industrial Internship** 09/2017—03/2018

Orochem Technologies, Inc, Naperville, IL, U.S.

Role: To use molecular simulations to increase the efficiency of industrial separations; to work with employees to help to facilitate SBIR project between IIT and Orochem Tech; to develop a software prototype for enantio-separation of chiral drugs.

**Undergraduate Research Assistant**

09/2011 - 05/2012

Sichuan University, Chengdu, Sichuan Province, China

Role: To synthesis and characterize organic fluorescent materials.

**TEACHING EXPERIENCE**

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**Teaching Assistant**

06/2015—08/2015

Illinois Institute of Technology, Chicago, IL, U.S.

Role: Supervised and guided laboratory work in fluid flow, heat transfer, distillation, humidification, drying, gas absorption, filtration, etc. in an undergraduate Unit Operations course in Chemical Engineering.

**Undergraduate Research Mentor**

Summer, 2021

University of Notre Dame, Notre Dame, IN, U.S.

Role: Trained summer graduate student on how to use molecular dynamics simulations to model ionic liquids and other systems of interest.

**SCIENTIFIC COMMUNITY AND OUTREACH ACTIVITIES**

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**Proposal Preparations**

- The Icelandic Research Fund (2022): Biochirality of usnic acid enantiomers in lichens (ChiralLichen).
- Air Liquid Project: Conversion of Ortho to Para Hydrogen.
- NSF: Using Machine Learning Technology to Extract and Study Phenomena That Are Not Well Understood in Molecular Modeling Simulations.
- GOALI: Molecular Dynamics Simulations for Prediction of Separation Factors for a Polysaccharide Chiral Stationary Phase in Enantiomeric Chromatographic Separations

**Manuscript Reviews**

- Adsorption.
- The Journal of Physical Chemistry
- Molecular Simulation
- Fluid Phase Equilibria

**AWARDS & HONORS**

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5. NSF Graduate Research Fellowship, Illinois Institute of Technology, 2015
4. Gamson Fellowship, Illinois Institute of Technology, 2014
3. Energy Technology Fellowship, Illinois Institute of Technology, 2013
2. Excellent Undergraduate Award, Sichuan University, 2010
1. Excellent Undergraduate Award, Sichuan University, 2009

## PUBLICATIONS

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14. **Xiaoyu Wang**, Yujia Wang, Rajamani Gounder, Edward Maginn, and William Schneider “Using Molecular Modeling Methods to Predict the Aluminum Distribution and Arrangement in the Chabazite Zeolite with the Presence of Organic Structure Directing Agents” (in preparation)
13. Derrick Poe, **Xiaoyu Wang**, Yong Zhang, Jeffery Klein, William Dean, Burcu Gurkan, and Edward J. Maginn, “A Systematic Study of Deep Eutectic Solvents Composed of Choline Chloride and Phenol Derivatives: A Combined Study of Experimental and Molecular Dynamics Simulation Methods” (in preparation)
12. **Xiaoyu Wang**, Cynthia J Jameson, Sohail Murad, “Molecular dynamics simulations of chiral recognition of drugs by amylose polymers coated on amorphous silica” *Molecular Physics* 2021, (in press, online available)
11. Cynthia J Jameson, **Xiaoyu Wang**, Sohail Murad, “Molecular Dynamics Simulations of Enantiomeric Separations as an Interfacial Process in HPLC” *AIChE Journal* 2021, 67, e17143
10. **Xiaoyu Wang**, Cynthia Jameson, Sohail Murad, “Modeling enantiomeric separations as an interfacial process using amylose tris(3,5-dimethylphenyl carbamate) (ADMPC) polymers coated on amorphous silica” *Langmuir* 2020, 36, 1113-1124
9. **Xiaoyu Wang**, Cynthia Jameson, Sohail Murad, “Interfacial Thermal Conductivity and its Anisotropy” *Processes* 2020, 8, 27
8. **Xiaoyu Wang**, David Venerus, Ishwar Puri, Sohail Murad, “On Using the Anisotropy in the Thermal Resistance of Solid-Fluid Interfaces to More Effectively Cool Nano-electronics” *Molecular Simulation* 2020, 46, 162-167
7. Xuerui Wang, Yuting Zhang, **Xiaoyu Wang**, Eduardo Andres-Garcia, Peng Du, Lorena Giordano, Lin Wang, Zhou Hong, Xuehong Gu, Sohail Murad, Freek Kapteijn, “Xe Recovery by DD3R Zeolite Membranes - Application in Anaesthetics” *Angewandte Chemie International Edition* 2019, 58, 15518-15525
6. **Xiaoyu Wang**, David House, Priyanka Oroskar, Anil Oroskar, Asha Oroskar, Cynthia Jameson, Sohail Murad, “Molecular Dynamics Simulations of the Chiral Recognition Mechanism for a Polysaccharide Chiral Stationary Phase in Enantiomeric Chromatographic Separations” *Molecular Physics* 2019, 117, 3569-3588
5. Kevin Hinkle, **Xiaoyu Wang**, Xuehong Gu, Cynthia Jameson, Sohail Murad, “Computational Molecular Modeling of Transport Processes in Nanoporous Membranes” *Processes* 2018, 6, 124
4. Chuan Chen, Yuli Cheng, Li Peng, Chun Zhang, Zhengqi Wu, Xuehong Gu, **Xiaoyu Wang**, Sohail Murad “Fabrication and stability exploration of hollow fiber mordenite zeolite membranes for isopropanol/water mixture separation” *Microporous and Mesoporous Materials* 2019, 274, 347-355
3. **Xiaoyu Wang**, Sohail Murad, “Molecular dynamics simulations of liquid-liquid phase equilibrium of ternary methanol/water/hydrocarbon mixtures” *Fluid Phase Equilibria* 2018, 470, 109-119
2. Binwu Zhao, Priyanka Sharma, **Xiaoyu Wang**, David House, Anil Oroskar, Asha Oroskar, Cynthia Jameson, Sohail Murad, “Computational study on chiral recognition of drug molecules” *Langmuir* 2017, 33, 11246-11256
1. Fanyu Qu, Rui Shi, Li Peng, Yuting Zhang, Xuehong Gu, **Xiaoyu Wang**, Sohail Murad, “Understanding the Effect of Zeolite Crystal Expansion/Contraction on Separation Performance of NaA Zeolite Membrane: A Combined Experimental and Molecular Simulation Study” *Journal of Membrane Science* 2017, 539, 14-23

## CONFERENCES

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7. “Using Molecular Simulations to Understand the Structure and Properties of Deep Eutectic Solvents, With Application to Flow Batteries.” V CINE-CMSC Workshop, Sao Carlos Institute of Chemistry, University of Sao Paulo, Sao Carlos, Brazil (Derrick Poe, Yong Zhang, **Andy Wang**, and Edward Maginn)
6. “On Using the Anisotropy in the Thermal Resistance of Solid-Fluid Interfaces to More Effectively Cool Nano-electronics.” Fundamental Research in Transport Processes, November 12, 2019, AIChE Annual Meeting, Orlando, FL. (co-authors: David Venerus, Ishwar Puri, Sohail Murad)

5. "Molecular simulations of separations of enantiomer using chiral stationary phases." Division of Colloid and Surface Chemistry, March 31st, 2019, ACS Spring 2019 National Meeting, Orlando, FL. (co-authors: Priyanka Sharma, Cynthia Jameson, Sohail Murad)
4. "Molecular dynamics simulations of liquid-liquid phase equilibrium of ternary methanol/water/hydrocarbon mixtures" March 14th, 2018, AIChE Midwest Regional Conference, Chicago. (co-author: Sohail Murad)
3. "Molecular Modeling as a Screening Tool to Separate Enantiomers of Chiral Compounds Using Polysaccharide-based Chiral Stationary Phases for Orphan Drugs" Feb 28th, 2017, AIChE Midwest Regional Conference, Chicago. (co-authors: Binwu Zhao, Priyanka Sharma, Cynthia Jameson, Sohail Murad)
2. "Molecular Modeling of Liquid-Liquid Phase Equilibria in Ternary Systems" March 1st, 2017, AIChE Midwest Regional Conference, Chicago. (co-author: Sohail Muard)
1. "Effect of Linear Hexane on Dehydration of Isopropanol-Water mixture through NaA Zeolite Membranes" March 3rd, 2016, AIChE Midwest Regional Conference, Chicago. (co-author: Sohail Murad)