BING YAN

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EDUCATION

New York University *Sep 2022 - Present*
Ph.D. in Computer Science
Advisors: Prof. Kyunghyun Cho
Thesis: Computational Molecule Design and Chemical Reaction Modeling

Massachusetts Institute of Technology *Sep 2014 - Jun 2019*
Ph.D. in Chemistry
Advisor: Prof. Yogesh Surendranath
Thesis: Designing Interfacial Structures for Selective Electrocatalysis

Peking University, China *Sep 2010 - Jul 2014*
B.S. in Chemistry
Advisor: Prof. Song Gao
Thesis: Synthesis and Properties of Dysprosium-based Single-Molecule Magnets
Graduated with **Highest Honor** (10 laureates every 2 years)

PROFESSIONAL APPOINTMENTS

Meta *Sep 2024 - Present*
Visiting Researcher
Mentor: Dr. Ricky Tian Qi Chen
Research Focus: Adjoint matching for molecule and material design

Massachusetts Institute of Technology *Aug 2019 - Aug 2022*
Postdoctoral Associate
Advisor: Prof. Yuriy Román, Department of Chemical Engineering
Research Focus: Electrochemical activation of C-C bonds for plastic and biomass deconstruction

PUBLICATIONS

13 **Bing Yan**, Benjamin K. Miller, Anuroop Sriram, Zachary Ulissi, Kyunghyun Cho, Ricky T. Q. Chen. "EVA-Flow: Environment-Aware Flow Matching for 3D Molecular Conformation Generation" *Submitted.*

12 Aaron J Havens, Benjamin K. Miller, **Bing Yan**, Carles Domingo-Enrich, Anuroop Sriram, Daniel S. Levine, Brandon M Wood, Bin Hu, Brandon Amos, Brian Karrer, Xiang Fu, Guan-Horng Liu, Ricky T. Q. Chen. "Adjoint Sampling: Highly Scalable Diffusion Samplers via Adjoint Matching" *ICML*, 2025.

11 **Bing Yan**, Angelica Chen, Kyunghyun Cho. "Inconsistency of LLMs in Molecular Representations" *Digital Discovery*, 2025, Advance Article.

10 **Bing Yan**, Kyunghyun Cho. "CatScore: Evaluating Asymmetric Catalyst Design at High Efficiency" *Digital Discovery*, 2024, Advance Article.

9 Siru Ouyang, Zhuosheng Zhang, **Bing Yan**, Xuan Liu, Jiawei Han, Lianhui Qin. "Structured Chemistry Reasoning with Large Language Models."*ICML*, 2024.

8 **Bing Yan**, Changxia Shi, Gregg T Beckham, Eugene Y.-X. Chen, Yuriy Román-Leshkov. "Electrochemical Activation of C-C Bonds via Mediated Hydrogen Atom Transfer Reactions" *ChemSusChem.*, 2022, 15, e2021023. *Very Important Paper*.

7 **Bing Yan**, Ryan P. Bisbey, Alexander Alabugin, Yogesh Surendranath. "Mixed Electron-Proton Conductors Enable Spatial Separation of Bond Activation and Charge Transfer in Electrocatalysis." *J. Am. Chem. Soc.*, 2019, 141, 11115-11122.

6 Youngmin Yoon, **Bing Yan**, Yogesh Surendranath. "Suppressing Ion Transfer Enables Versatile Measurements of Electrochemical Surface Area for Intrinsic Activity Comparisons." *J. Am. Chem. Soc.*, 2018, 140, 2397-2400.

5 **Bing Yan**, Nolan M. Concannon, Jarrod D. Milshtein, Fikile R. Brushett, Yogesh Surendranath. **Inside Cover**: "A Membrane-Free Neutral pH Formate Fuel Cell Enabled by a Selective Ni_3S_2 Oxygen Reduction Catalyst." *Angew. Chem. Int. Ed.*, 2017, 56, 7496-7499.

4 **Bing Yan**, Dilip Krishnamurthy, Christopher H. Hendon, Siddharth Deshpande, Yogesh Surendranath, Venkatasubramanian Viswanathan. "Surface Restructuring of Nickel Sulfide Generates Optimally Coordinated Active Sites for Oxygen Reduction Catalysis." *Joule*, 2017, 1, 600-612. (**Referred to by** Fang Song, Jordan Katz, Xile Hu. "Catalyst Surface Dynamics Reveals a Simple Geometric Descriptor of Activity" *Joule*, 2017, 1, 421-430.)

3 Wen-Bin Sun, **Bing Yan**, Li-Hui Jia, Bing-Wu Wang, Qian Yang, Xin Cheng, Hong-Feng Li, Peng Chen, Zhe-Ming Wang, Song Gao. "Dinuclear Dysprosium SMMs Bridged by a Neutral Bipyrimidine Ligand: Two Crystal Systems that Depend on Different Lattice Solvents Lead to a Distinct Slow Relaxation Behavior." *Dalton Trans.*, 2016, 45, 8790-8794.

2 Joseph M. Falkowski, Nolan M. Concannon, **Bing Yan**, Yogesh Surendranath. "Heazlewoodite, Ni_3S_2: A Potent Catalyst for Oxygen Reduction to Water under Benign Conditions." *J. Am. Chem. Soc.*, 2015, 137, 7978-7981.

1 Wen-Bin Sun, **Bing Yan**, Yi-Quan Zhang, Bing-Wu Wang, Zhe-Ming Wang, Jun-Hua Jia, Song Gao. "The Slow Magnetic Relaxation Regulated by Ligand Conformation of a Lanthanide Single-Ion Magnet $[Hex_4N][Dy(DBM)_4]$." *Inorg. Chem. Front.*, 2014, 1, 503-509.

PROFESSIONAL SERVICE

Area Chair for NeurIPS AI for Science Workshop	2025
Reviewer for ACL	2025
Organizer for NYU CILVR Seminar Series	2023-2025
Reviewer for ICLR, ACL	2024
Area Chair for ICML AI for Science Workshop	2024

Reviewer for EMNLP 2023

Organizer for NYU AI School 2023

AIChE Young Professional volunteer 2021

Reviewer for Journal of Nanotechnology 2018

Reviewer for Chemistry of Materials 2017

AWARDS & HONORS

Henry M. MacCracken Fellowship (full graduate funding) 2022-2027

Rowland Fellowship finalist 2021

Moore Fellowship 2018

Women in Chemistry Professional Development Grant 2017

Dow Chemistry scholarship 2013

Hui-Chun Chin and Tsung-Dao Lee Chinese Undergraduate Research Endowment 2013

National Fund for Fostering Talents of Basic Sciences (NSFC J1030413) 2013

Merit Student of Beijing (top 1%) 2012

SK scholarship 2012

Canon scholarship 2011

TALKS & POSTERS

5th meeting for GRP Materials Discovery: "nconsistency of LLMs in Molecular Representations." Feb 2025, Remote

2021 AIChE Annual Meeting (Oral): "Mediated Oxidative Carbon-Carbon Bond Activation and Application to Polystyrene Decomposition." Nov 2021, Boston

MIT Chemistry Student Seminar (Oral): "Selective Oxygen Reduction and Hydrogen Oxidation Catalysis for Fuel Cells." May 2018, Cambridge

Electrochemistry Gordon Research Seminar & Conference (Oral): "Exploiting Hydrogen Spillover for Selective Electrocatalysis." Jan 2018, Ventura

Sixth Annual C3E Women in Clean Energy Symposium (Poster): "Selective Cathode and Anode Electrocatalysis for Membrane-Free Fuel Cells." Nov 2017, Cambridge

The 68th Annual Meeting of the International Society of Electrochemistry (Oral): "Oxygen Reduction Catalyst Ni_3S_2 Oxidative Surface Restructuring and Application in Membrane-Free Fuel Cells." Aug 2017, Providence

Nanomaterials for Applications in Energy Technology Gordon Research Seminar and Conference (Poster): "ORR Catalyst Ni_3S_2 Oxidative Surface Restructuring and Application in Mixed-Reactant Fuel Cells." Feb 2017, Ventura

250th ACS National Meeting (Poster): "Transition Metal Chalcogenide Nanofilms: Oxygen Reduction Reaction Catalysts Prepared by E-ALD." Aug 2015, Boston

TEACHING

Teaching Assistant

Machine Learning	Dec 2024 - May 2025
Principle of Inorganic Chemistry II	Aug - Dec 2015
Organic & Inorganic Laboratory	Aug - Dec 2014