Bing Yan

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Research Interests

I combine experimental catalysis and electrochemistry with machine learning to understand and control chemical reactivity. I will develop models that predict reaction pathways and rates from molecular structures and reaction conditions, then use these predictions to design catalysts and electrochemical interfaces for new substrates. I will also identify untargeted products from NMR and mass spectra, then investigate how they form to uncover missing reactions and improve catalyst and condition design.

Education and Postdoctoral Training

New York University 2022–2027 expected
PhD in Computer Science
Advisor: Kyunghyun Cho
Dissertation: *Computational Molecule Design and Chemical Reaction Modeling*

Massachusetts Institute of Technology 2019–2022
Postdoctoral Associate, Department of Chemical Engineering
Advisor: Yuriy Román-Leshkov
Project: *Electrochemical C–C bond activation for plastic and biomass deconstruction*

Massachusetts Institute of Technology 2014–2019
PhD in Chemistry
Advisor: Yogesh Surendranath
Dissertation: *Designing Interfacial Structures for Selective Electrocatalysis*

Peking University 2010–2014
BS in Chemistry
Advisor: Song Gao
Dissertation: *Synthesis and Properties of Dysprosium-based Single-Molecule Magnets*
Graduated with **Highest Honor** (one of 10 recipients selected university-wide every two years)

Research and Professional Appointments

Matterstack, Inc., Research Consultant September 2026–present
Manager: Stefano Martiniani
Project: *Developing scientific agents for materials discovery*

Meta FAIR, Visiting Researcher September 2024–August 2026
Managers: Benjamin K. Miller and Ricky T. Q. Chen
Project: *Generative modeling for molecules and reactions*

Peer-Reviewed Publications

1. **Bing Yan**, Anuroop Sriram, Zachary W. Ulissi, Kyunghyun Cho, Ricky T. Q. Chen, and Benjamin K. Miller. "EVA-Flow: Learning Shared Chemistry for Unified Environment-Aware Molecular Conformation Generation." *Transactions on Machine Learning Research*, 2026.
2. **Bing Yan**, Gregory Wolfe, Stefano Martiniani, and Kyunghyun Cho. "AskChem: Claim-Centered Infrastructure for Chemistry Literature Synthesis." *EMNLP System Demonstrations*, 2026.
3. **Bing Yan**, Ge Sun, Juan J. de Pablo, Stefano Martiniani, and Kyunghyun Cho. "ReasonFlow: Flow Matching that Thinks Step by Step." *Findings of the Association for Computational Linguistics: EMNLP*, 2026.

4. 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[*], and Ricky T. Q. Chen[*]. "Adjoint Sampling: Highly Scalable Diffusion Samplers via Adjoint Matching." *ICML*, 2025. [*]*Core contributors.*
5. **Bing Yan**, Angelica Chen, and Kyunghyun Cho. "Inconsistency of LLMs in Molecular Representations." *Digital Discovery* 4, 2876–2892, 2025.
6. **Bing Yan** and Kyunghyun Cho. "CatScore: Evaluating Asymmetric Catalyst Design at High Efficiency." *Digital Discovery* 3, 1624–1637, 2024.
7. Siru Ouyang, Zhuosheng Zhang, **Bing Yan**, Xuan Liu, Yejin Choi, Jiawei Han, and Lianhui Qin. "Structured Chemistry Reasoning with Large Language Models." *International Conference on Machine Learning*, 2024.
8. **Bing Yan**, Changxia Shi, Gregg T. Beckham, Eugene Y.-X. Chen, and Yuriy Román-Leshkov. "Electrochemical Activation of C–C Bonds through Mediated Hydrogen Atom Transfer Reactions." *ChemSusChem* 15, e202102317, 2022. Very Important Paper.
9. **Bing Yan**, Ryan P. Bisbey, Alexander Alabugin, and Yogesh Surendranath. "Mixed Electron–Proton Conductors Enable Spatial Separation of Bond Activation and Charge Transfer in Electrocatalysis." *Journal of the American Chemical Society* 141, 11115–11122, 2019.
10. Youngmin Yoon, **Bing Yan**, and Yogesh Surendranath. "Suppressing Ion Transfer Enables Versatile Measurements of Electrochemical Surface Area for Intrinsic Activity Comparisons." *Journal of the American Chemical Society* 140, 2397–2400, 2018.
11. **Bing Yan**, Dilip Krishnamurthy, Christopher H. Hendon, Siddharth Deshpande, Yogesh Surendranath, and Venkatasubramanian Viswanathan. "Surface Restructuring of Nickel Sulfide Generates Optimally Coordinated Active Sites for Oxygen Reduction Catalysis." *Joule* 1, 600–612, 2017. Discussed in a *Joule* commentary (2017).
12. **Bing Yan**, Nolan M. Concannon, Jarrod D. Milshtein, Fikile R. Brushett, and Yogesh Surendranath. "A Membrane-Free Neutral pH Formate Fuel Cell Enabled by a Selective Nickel Sulfide Oxygen Reduction Catalyst." *Angewandte Chemie International Edition* 56, 7496–7499, 2017. Inside Cover.
13. Wen-Bin Sun, **Bing Yan**, Li-Hui Jia, Bing-Wu Wang, Qian Yang, Xin Cheng, Hong-Feng Li, Peng Chen, Zhe-Ming Wang, and 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 Transactions* 45, 8790–8794, 2016.
14. Joseph M. Falkowski, Nolan M. Concannon, **Bing Yan**, and Yogesh Surendranath. "Heazlewoodite, Ni_3S_2: A Potent Catalyst for Oxygen Reduction to Water under Benign Conditions." *Journal of the American Chemical Society* 137, 7978–7981, 2015.
15. Wen-Bin Sun, **Bing Yan**, Yi-Quan Zhang, Bing-Wu Wang, Zhe-Ming Wang, Jun-Hua Jia, and Song Gao. "The Slow Magnetic Relaxation Regulated by Ligand Conformation of a Lanthanide Single-Ion Magnet $[Hex_4N][Dy(DBM)_4]$." *Inorganic Chemistry Frontiers* 1, 503–509, 2014.

Manuscripts in Preparation

Bing Yan, Zachary Ulissi, Benjamin Kurt Miller, and Kyunghyun Cho. "SPARK: Learning unseen chemistry to plan experiments." Manuscript in preparation.

Selected Software, Data, and Research Infrastructure

AskChem — https://askchem.org
Claim-centered scientific-literature infrastructure with millions of source-linked claims from approximately 147,000 papers: a graph of claims and source passages, AskChem-Bench, dataset, web interface, REST API, SDK, and MCP server. Source: GitHub repo. Dataset: Hugging Face.
Featured by the NYU Center for Data Science, October 23, 2026 (research blog and X announcement).

SPARK — https://huggingface.co/spaces/bing-yan/spark
Simulation-based inference framework, reaction-network simulator, trained models, and electrochemical data for mechanism and kinetic-parameter inference.

CatScore — github.com/bingyan4science/CatScore
Learned evaluation metric and code for asymmetric-catalyst design.

Molecular Representation Consistency — github.com/bingyan4science/consistency
Code and data for evaluating the consistency of language-model predictions across equivalent molecular representations.

Fellowships, Scholarships, and Research Support

- Meta AI Mentorship Program (AIM), 2024–2026.
- Henry M. MacCracken Fellowship, New York University, 2022–2027.
- 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, 2013.
- SK Scholarship, 2012.
- Canon Scholarship, 2011.

Awards and Honors

- Gold Reviewer, ICML, 2026.
- Poster Award, Gordon Research Conference on AI for Materials, Energy, and Chemical Sciences, 2026.
- Rowland Fellowship finalist, 2021.
- Graduated with Highest Honor, Peking University, 2014.
- Merit Student of Beijing, top 1%, 2012.

Teaching and Mentoring

Teaching Assistant

- **Machine Learning (CSCI-GA 2565)**, New York University, Fall 2026.
  Teaching assistant for Kyunghyun Cho's graduate course. Provide weekly office hours and support course assessment, including the first in-person examination.
- **Fundamentals of Machine Learning (CSCI-UA 473)**, New York University, Spring 2026.
  Teaching assistant for an undergraduate machine learning course.
- **Introduction to Machine Learning**, New York University, December 2024–May 2025.
  Held office hours, graded and provided feedback, led recitation/review sessions, and delivered guest lectures.

- **Principles of Inorganic Chemistry II**, Massachusetts Institute of Technology, August–December 2015.
- **Organic and Inorganic Laboratory**, Massachusetts Institute of Technology, August–December 2014.

Undergraduate Mentoring

- **Alexander Alabugin**, June–August 2017. Provided technical training and support for scientific writing and presentation.
- **Nolan M. Concannon**, June 2015–December 2016. Provided technical training and support for scientific writing and presentation.

Educational and Research Community Organization

- Organizer, NYU CILVR Seminar Series, 2023–2025.
- Organizer and instructor, NYU AI School, 2023. Helped develop the curriculum and technical program and contributed instruction for a free introductory school serving early undergraduates, including students outside computing disciplines.

Professional Service

- **Area Chair:** ICML AI4Science Workshop (2026), NeurIPS AI for Science Workshop (2025), and ICML AI for Science Workshop (2024).
- **Reviewer:** NeurIPS, ICML, ICLR, ACL, EMNLP Demo, AAAI, TMLR, and COLM (2026). ACL (2025), ICLR and ACL (2024), EMNLP (2023), *Journal of Nanotechnology* (2018), and *Chemistry of Materials* (2017).
- **Volunteer:** AIChE Young Professionals, 2021.

Outreach

- Co-presenter, "Beyond ChatGPT: What Else Can AI Become?" Vision 2026 STEAM Conference, October, 2026. Introduced high-school students to AI for chemical discovery through demonstrations of AskChem and SPARK, connecting chemistry literature, reaction mechanisms, and experiment selection.
- NetPals STEM Explorations Club, Putnam Avenue Upper School, January–May 2021. Designed activities, facilitated sessions, and coordinated with teachers and volunteers.
- STEM outreach, East Boston Public High School, 2015–2019. Designed activities, facilitated sessions, and coordinated with teachers and volunteers.

Selected Presentations

Talks and Seminars

- "SPARK: Simulation-based Posterior Amortisation for Reaction Kinetics." Meta FAIR Chemistry Team Reading Group, April 2026. *Invited talk.*
- "From Tokens to Coordinates: Do Molecular Models Really Understand Chemistry?" Global AI Frontier Lab, NYU, December 2025. *Invited talk.*
- "Inconsistency of LLMs in Molecular Representations." GRP Materials Discovery meeting, February 2025. *Invited talk.*
- "Mediated Oxidative Carbon–Carbon Bond Activation and Application to Polystyrene Decomposition." AIChE Annual Meeting, November 2021.
- "Selective Oxygen Reduction and Hydrogen Oxidation Catalysis for Fuel Cells." MIT Chemistry Student Seminar, May 2018. *Invited talk.*

- "Exploiting Hydrogen Spillover for Selective Electrocatalysis." Electrochemistry Gordon Research Seminar and Conference, January 2018. *Late-Breaking Topics*, talk selected from poster presentations.
- "Oxygen Reduction Catalyst Ni_3S_2 Oxidative Surface Restructuring and Application in Membrane-Free Fuel Cells." International Society of Electrochemistry Annual Meeting, August 2017.

Posters and Demonstrations

- "AI-Guided Mechanism Inference and Experiment Design in Catalytic and Electrochemical Systems." Meet the Faculty Poster Session, AIChE Annual Meeting, Minneapolis, November 2026.
- "ReasonFlow: Flow Matching that Thinks Step by Step." EMNLP 2026, Budapest, Hungary, October 2026.
- "AskChem: Claim-Centered Infrastructure for Chemistry Literature Synthesis." EMNLP 2026 System Demonstrations, Budapest, Hungary, October 2026. *Poster and demonstration.*
- "EVA-Flow: Learning Shared Chemistry for Unified Environment-Aware Molecular Conformation Generation." Gordon Research Conference AI for Materials, Energy, and Chemical Sciences, February 2026.
- "Selective Cathode and Anode Electrocatalysis for Membrane-Free Fuel Cells." C3E Women in Clean Energy Symposium, November 2017.

Referees

Yogesh Surendranath yogi@mit.edu
Professor of Chemistry and Chemical Engineering, Massachusetts Institute of Technology
Doctoral advisor (Chemistry)

Yuriy Román-Leshkov yroman@mit.edu
Professor of Chemical Engineering, Massachusetts Institute of Technology
Postdoctoral advisor

Kyunghyun Cho kyunghyun.cho@nyu.edu
Professor of Computer Science and Data Science, New York University
Doctoral advisor (Computer Science)