

Bing Yan

bing.yan@nyu.edu · <https://bingyan.me> · Google Scholar

Background

New York University PhD in Computer Science Advisor: Kyunghyun Cho Dissertation: <i>Computational Molecule Design and Chemical Reaction Modeling</i>	2022–2027 expected
Massachusetts Institute of Technology, Department of Chemical Engineering Postdoctoral Associate Advisor: Yuriy Román-Leshkov Project: <i>Electrochemical C–C bond activation for plastic and biomass deconstruction</i>	2019–2022
Massachusetts Institute of Technology PhD in Chemistry Advisor: Yogesh Surendranath Dissertation: <i>Designing Interfacial Structures for Selective Electrocatalysis</i>	2014–2019
Peking University BS in Chemistry Advisor: Song Gao Dissertation: <i>Synthesis and Properties of Dysprosium-based Single-Molecule Magnets</i> Graduated with Highest Honor (one of 10 recipients selected university-wide every two years)	2010–2014

Research and Professional Appointments

Meta FAIR, Visiting Researcher Mentors: Benjamin K. Miller and Ricky T. Q. Chen Project: <i>Generative modeling for molecules and reactions</i>	September 2024–August 2026
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Research Interests

World models for experimental discovery: generative and probabilistic models that combine scientific knowledge with experimental data, identify and repair model errors, and select informative experiments. Applications span electrochemical and catalytic reaction systems, with foundations in mechanism inference, molecular generation, and scientific NLP.

Peer-Reviewed Publications

1. **Bing Yan**, Gregory Wolfe, Stefano Martiniani, and Kyunghyun Cho. “AskChem: Claim-Centered Infrastructure for Chemistry Literature Synthesis.” *EMNLP System Demonstrations*, 2026.
2. **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.
3. 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-Hong Liu, and Ricky T. Q. Chen. “Adjoint Sampling: Highly Scalable Diffusion Samplers via Adjoint Matching.” *International Conference on Machine Learning*, 2025.
4. **Bing Yan**, Angelica Chen, and Kyunghyun Cho. “Inconsistency of LLMs in Molecular Representations.” *Digital Discovery*, 2025.
5. **Bing Yan** and Kyunghyun Cho. “CatScore: Evaluating Asymmetric Catalyst Design at High Efficiency.” *Digital Discovery*, 2024.
6. 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.

7. **Bing Yan**, Changxia Shi, Gregg T. Beckham, Eugene Y.-X. Chen, and Yuriy Román-Leshkov. “Electrochemical Activation of C–C Bonds via Mediated Hydrogen Atom Transfer Reactions.” *ChemSusChem* 15, e202102317, 2022. Very Important Paper.
8. **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.
9. 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.
10. **Bing Yan**, Dilip Krishnamurthy, Christopher H. Hendon, Siddharth Deshpande, and Yogesh Surendranath. “Surface Restructuring of Nickel Sulfide Generates Optimally Coordinated Active Sites for Oxygen Reduction Catalysis.” *Joule* 1, 600–612, 2017. (Referred to by Fang Song, Jordan Katz, Xile Hu. “Catalyst Surface Dynamics Reveals a Simple Geometric Descriptor of Activity” *Joule*, 2017, 1, 421-430.)
11. **Bing Yan**, Nolan M. Concannon, and Yogesh Surendranath. **Inside Cover**: “A Membrane-Free Neutral-pH Formate Fuel Cell Enabled by a Selective Ni₃S₂ Oxygen Reduction Catalyst.” *Angewandte Chemie International Edition* 56, 7496–7499, 2017. Inside Cover.
12. 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.
13. Joseph M. Falkowski, Nolan M. Concannon, **Bing Yan**, and Yogesh Surendranath. “Heazlewoodite, Ni₃S₂: A Potent Catalyst for Oxygen Reduction to Water under Benign Conditions.” *Journal of the American Chemical Society* 137, 7978–7981, 2015.
14. 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 [Hex₄N][Dy(DBM)₄].” *Inorganic Chemistry Frontiers* 1, 503–509, 2014.

Manuscripts Under Review and in Preparation

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.” Under review at TMLR.

Bing Yan, Lavender Yao Jiang, and Kyunghyun Cho. “Toward Discrete-Internals Transformers.” Under review at NeurIPS 2026.

Bing Yan, Zachary Ulissi, Benjamin Kurt Miller, and Kyunghyun Cho. “SPARK: Calibrated Neural Inference for Reaction Mechanisms and Kinetics.” Manuscript in preparation.

Selected Software, Data, and Research Infrastructure

AskChem — <https://askchem.org>

Claim-centered scientific-literature infrastructure with 2.4 million source-linked claims from 147,000 papers; includes an evidence graph, AskChem-Bench, open dataset, web interface, REST API, SDK, and MCP server. Source: [GitHub repo](#). Dataset: [Hugging Face](#).

SPARK — <https://huggingface.co/spaces/bing-yan/spark>

Simulation-based inference framework, reaction-network simulator, trained models, and electrochemical data for calibrated mechanism 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 testing whether language-model predictions remain stable across equivalent molecular representations.

Awards and Honors

- Gold Reviewer, ICML, 2026.
- Poster Award, Gordon Research Conference on AI for Materials, Energy, and Chemical Sciences, 2026.
- Henry M. MacCracken Fellowship, New York University, 2022–2027.
- Rowland Fellowship finalist, 2021.
- Moore Fellowship, 2018.
- Women in Chemistry Professional Development Grant, 2017.
- Graduated with Highest Honor, Peking University, 2014.
- 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.
- Merit Student of Beijing, top 1%, 2012.
- SK Scholarship, 2012.
- Canon Scholarship, 2011.

Teaching and Mentoring

Teaching Assistant

- 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 select topics, design the curriculum, organize speakers and the technical program, and contribute instruction or instructional materials.

Professional Service

- Area Chair, ICML AI4Science Workshop, 2026.
- Reviewer, NeurIPS, ICML, ICLR, ACL, EMNLP Demo, AAAI, TMLR, COLM, 2026.
- Area Chair, NeurIPS AI for Science Workshop, 2025.
- Reviewer, ACL, 2025.
- Area Chair, ICML AI for Science Workshop, 2024.

- Reviewer, ICLR and ACL, 2024.
- Reviewer, EMNLP, 2023.
- AIChE Young Professionals volunteer, 2021.
- Reviewer, *Journal of Nanotechnology*, 2018.
- Reviewer, *Chemistry of Materials*, 2017.

Outreach

- NetPals STEM Explorations Club, Putnam Avenue Upper School, January–May 2021. Designed or adapted activities, facilitated sessions, and coordinated with teachers or volunteers.
- STEM outreach, East Boston Public High School, 2015–2019. Designed or adapted activities, facilitated sessions, and coordinated with teachers or volunteers.

Selected Talks and Presentations

- “AI-Guided Mechanism Inference and Experiment Design In Catalytic and Electrochemical Systems.” AIChE Annual Meeting, November 2026.
- “SPARK: Simulation-based Posterior Amortisation for Reaction Kinetics.” Meta FAIR Chemistry Team Reading Group, April 2026.
- “EVA-Flow: Learning Shared Chemistry for Unified Environment-Aware Molecular Conformation Generation.” Gordon Research Conference AI for Materials, Energy, and Chemical Sciences, February 2026.
- “From Tokens to Coordinates: Do Molecular Models Really Understand Chemistry?” Global AI Frontier Lab, NYU, December 2025.
- “Inconsistency of LLMs in Molecular Representations.” GRP Materials Discovery meeting, February 2025.
- “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.
- “Exploiting Hydrogen Spillover for Selective Electrocatalysis.” Electrochemistry Gordon Research Seminar and Conference, January 2018.
- “Selective Cathode and Anode Electrocatalysis for Membrane-Free Fuel Cells.” C3E Women in Clean Energy Symposium, November 2017.
- “Oxygen Reduction Catalyst Ni_3S_2 Oxidative Surface Restructuring and Application in Membrane-Free Fuel Cells.” International Society of Electrochemistry Annual Meeting, August 2017.

Referees

Kyunghyun Cho

Professor of Computer Science and Data Science, New York University

kyunghyun.cho@nyu.edu

Yogesh Surendranath

Professor of Chemistry, Massachusetts Institute of Technology

yogi@mit.edu

Benjamin K. Miller

Research Scientist, FAIR Chemistry, Meta

bkmi@meta.com