ACHYUT RANJAN GOGOI

Experimental & Computational Organic Chemist | PhD Candidate

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PROFILE

PhD Chemist with strong training in synthetic organic chemistry, catalytic reaction development, and computational mechanistic studies (DFT & MD), integrating experimentation and computation to solve complex challenges in drug discovery, process development, and predictive reaction design. Proven track record of **18+ peer-reviewed publications** in premier journals (Nature Catalysis, Nature Synthesis, JACS etc.) through productive collaborations with **10+** leading research groups globally. Expertise in bridging computational predictions with experimental validation to solve complex chemical challenges in asymmetric catalysis, reaction optimization, and mechanism-driven drug discovery.

RESEARCH EXPERIENCE

Visiting Graduate Researcher | University of California, Los Angeles
June 2025 – Present | Advisor: Prof. Osvaldo Gutierrez

Challenge: Iron-catalyzed asymmetric cross-electrophile coupling reactions were constrained by narrow substrate scopes requiring distinct synthetic strategies for different alkene classes & syringe-pump-based slow addition of the nucleophile, limiting their practicality for pharmaceutical applications.
Action: Led a five-member graduate research team to develop a novel iron-catalyzed reductive cross-coupling methodology by integrating high-throughput experimentation (HTE) with DFT-guided catalyst screening, enabling the design of a general synthetic strategy applicable across diverse alkene classes.
Results:

- Enabled reactivity across multiple previously inaccessible alkene classes, significantly broadening synthetic utility for drug discovery applications
- Developed a one-step, one-pot protocol that eliminates the need for syringe-pump-based slow addition, improving operational simplicity & pharmaceutical relevance
- Implemented a data-driven reaction design workflow combining HTE with computational validation to accelerate catalyst screening and reaction optimization

PhD Research | Texas A&M University
August 2021 – Present | Advisor: Prof. Osvaldo Gutierrez

Project 1: Iron-Catalyzed Asymmetric Multicomponent Cross-Coupling
Challenge: Existing methods for iron catalyzed asymmetric multicomponent cross-coupling reactions achieved only ~90% enantioselectivity & generated hard-to-remove phosphine oxide byproducts, limiting their pharmaceutical applications.
Action: Developed a sustainable phosphine free iron catalytic system by integrating DFT-guided mechanistic prediction, iterative synthetic optimization, and Mössbauer spectroscopic validation of catalytically active species.
Results:

- Achieved >98% enantioselectivity within 1 hour, surpassing precious-metal catalysts while reducing reaction time from 12 hours to 1 hour (~92% reduction)
- Developed methodology from proof-of-concept (mg scale) to preparative (gram scale), demonstrating scalability and operational relevance for process chemistry
- Established a phosphine-free, practical asymmetric process that eliminated phosphine oxide byproduct, simplifying reaction purification and improving sustainability
- Identified & characterized stereodetermining iron species through combined computational and Mössbauer spectroscopic analysis that guided the design of next generation iron-based asymmetric catalysts

Project 2: Collaborative Mechanism Elucidation Studies
Challenge: Complex catalytic transformations across multiple metal and photocatalytic systems lacked in-depth mechanistic understanding, limiting rational catalyst design and systematic performance improvement.
Action: Led DFT- and molecular-dynamics-based mechanistic investigations across multiple collaborative projects, working closely with experimental teams at 10+ institutions worldwide, including ICIQ, UChicago, Northwestern, Oxford, UW–Madison, NUS, University of Michigan and the University of Münster.
Results:

- Co-authored 18+ high-impact publications elucidating reaction mechanisms across iron, nickel, palladium, rhodium, light-mediated and metal-free catalytic systems
- Delivered actionable mechanistic insights that directly guided catalyst selection, reaction optimization and substrate scope expansion in partner laboratories
- Collaborated closely with interdisciplinary teams to develop computational mechanistic workflows adopted and cited by multiple research groups, supporting reproducible, data-driven decision-making in reaction optimization

Visiting Graduate Researcher | University of Oxford, United Kingdom
September 2023 – November 2023 | Advisor: Prof. Michael Neidig

Challenge: The active chiral catalytic species in iron-catalyzed asymmetric cross-coupling remained unidentified, limiting rational catalyst design and slowing rational optimization of enantioselectivity.
Action: Conducted systematic Mössbauer spectroscopy studies on transient iron intermediates to identify oxidation states and coordination environments of catalytically active chiral iron species.
Results:

- Successfully identified and characterized stereodetermining iron species, providing direct spectroscopic evidence of active catalyst structure and its role in stereocontrol
- Generated mechanistic insights that guided development of next-generation iron catalysts with improved selectivity
- Established spectroscopic benchmarks to support reproducible catalyst characterization and informed future mechanism guided discovery and modeling efforts

EDUCATION

PhD in Chemistry | Texas A&M University | 2021 – May 2026 (Expected) | GPA: 3.75
Focus: Computational Organic Chemistry & Asymmetric Iron Catalysis

M.Sc. in Chemistry | Indian Institute of Technology (IIT) Bombay | 2021 | CPI: 9.69/10.0

B.Sc. in Chemistry | University of Delhi | 2019 | CPI: 9.59/10.0

SELECTED PUBLICATIONS

Author of 18 peer-reviewed articles (2 first-author, 8 second-author publications) in premier journals including Nature Catalysis, Nature Communications, JACS, ACS Catalysis, Chem, and Angewandte Chemie. Two additional first-author manuscripts under review.

1. **Gogoi, A. R.**; Rentería-Gómez, A.; Tan, T.D.; Ng, J. W.; Koh, M. J.; Gutierrez, O. Iron-catalyzed radical difunctionalization of alkenes. *Nat. Synth.* **2025**, *4*, 1036–1055.
2. **Gogoi, A. R.**[#]; Usman, F. O.[#]; Mixdorf, J. C.; Gutierrez, O.; Nguyen, H. M. Rhodium-catalyzed Asymmetric Synthesis of 1,2-disubstituted Allylic Fluorides. *Angew. Chem. Int. Ed Engl.* **2023**, *62*.
3. Targos, K.; **Gogoi, A. R.**; Rentería-Gómez, Á.; Kim, M. J.; Gutierrez, O.; Wickens, Z. K. Mechanism of *Z*-Selective Allylic Functionalization via Thianthrenium Salts. *J. Am. Chem. Soc.* **2024**, *146*, 13689–13696.

Complete publication list https://achyutrgogoi.github.io/

SELECTED PRESENTATIONS & AWARDS

Sharon Dabney Memorial Scholarship – For excellence in research and departmental leadership (Texas A&M University)

SACNAS Diversity in Science Symposium (2023) – **Poster Award**

ACS Division of Organic Chemistry Graduate Research Symposium (San Diego, 2025) – Oral Presentation

ACS Fall National Meeting (Denver, 2024) – Oral Presentation

Gordon Research Conference (Physical Organic Chemistry, 2023) – Poster Presentation

Catalysis Innovation Consortium Systemwide Meeting (2025) – Virtual Oral Presentation

TECHNICAL PROFICIENCIES

Synthetic: Organic Synthesis | Asymmetric Catalysis | Organometallic Synthesis | High-Throughput Experimentation (HTE) | Air-Sensitive Chemistry (Schlenk & Glovebox) | Multi-Step Synthesis | Purification & Characterization

Computational: DFT (Gaussian, ORCA, GAMESS) | Molecular Dynamics | Python | C++ | Data Analysis & Visualization | Reaction Mechanism Elucidation | Catalyst Design | Structure-Activity Relationship (SAR)

Analytical: Mössbauer Spectroscopy | NMR (^{1}H, ^{13}C, RI-NMR) | FT-IR | UV-Vis | Chromatography (GC, HPLC)

Other: Cross-Functional Collaboration | Scientific Communication | Project Management | Mentorship

LEADERSHIP & OUTREACH

Secretary, Phi Lambda Upsilon Chemistry Honor Society, Texas A&M University

Co-Lead Instructor, *i*Carbon Computational Chemistry Initiative: Designed and delivered weekly workshops on DFT and molecular modeling, expanding STEM access for 15+ students from Sacramento City College and Long Beach City College

Physical Chemistry Division Representative, Chemistry Student Safety Committee, Texas A&M University

Student Ambassador, Catalysis Innovation Consortium (CIC) | Active ACS Member & Peer Reviewer

Recruitment Team Member, Texas A&M Chemistry Department Graduate Recruitment & Open House