ACHYUT RANJAN GOGOI

PhD Candidate in Chemistry (Computational Organic & Iron Catalysis)

Texas A&M University | Anticipated Graduation: May 2026

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SUMMARY

PhD candidate in Chemistry with **4+ years** of experience integrating computational modeling, synthetic methodology, and spectroscopy. Demonstrated excellence through **18+ high-impact publications** and international collaborative research with leading groups across **10+** universities. Expertise in organic synthesis, iron-catalyzed asymmetric cross-coupling, quantum chemical simulations (**DFT/MD**), data-driven catalyst design, high-throughput experimentation (**HTE**) and mechanism-guided reaction development. Passionate about applying computational chemistry and mechanistic insight to accelerate data-rich experimentation and sustainable catalysis.

RESEARCH EXPERIENCE

❖ **Visiting Graduate Researcher, UCLA (June'2025- Present)**

Project: Development of Iron Catalyzed Asymmetric Reductive Alkene Dicarbofunctionalization using High Throughput Experimentation (HTE) and DFT

Supervisor: Prof. Osvaldo Gutierrez, University of California, Los Angeles

Challenge: Asymmetric reductive alkene dicarbofunctionalization reactions are constrained by narrow substrate scopes requiring distinct synthetic strategies for different alkene classes and syringe-pump-based slow addition of the nucleophile in case of iron based dicarbofunctionalization strategies, limiting their practicality for pharmaceutical applications.

Action: Led a five-member graduate research team to develop an iron-catalyzed reductive alkene dicarbofunctionalization 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 pharmaceutical applications
- Developed a one-step, one-pot protocol that eliminates the need for syringe-pump-based slow addition, improving operational simplicity & pharmaceutical relevance

❖ **PhD Research, TAMU (August'2021-Present)**

Project 1: Mechanistic Insight Guided Rational Design of Iron-Catalyzed Asymmetric Multicomponent Cross-Coupling Strategies

Supervisor: Prof. Osvaldo Gutierrez, Texas A&M University

Challenge: Existing methods for iron catalyzed asymmetric multicomponent cross-coupling reactions achieved only ~82% enantiomeric excess (e.e.) and generated hard-to-remove phosphine oxide byproducts, limiting their pharmaceutical applications.

Action: Developed a sustainable phosphine-free iron-based catalytic system by integrating DFT-guided mechanistic prediction, iterative synthetic optimization, and Mössbauer spectroscopic identification of catalytically active species.

Results:

- Achieved >98% enantiomeric excess (e.e.) within 1 hour, surpassing previous literature precedents while reducing reaction time from ~12 hours, typical of nickel-based systems, to 1 hour
- 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: Harnessing the Symbiotic Potential of Computation & Experiment in Elucidation of Reaction Mechanisms

Supervisor: Prof. Osvaldo Gutierrez, Texas A&M University

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 the Martin group (ICIQ), Fleming group (Drexel), Scheidt group (Northwestern), Thomas and Powers groups (Texas A&M), Levin group (Chicago), and Wickens group (Wisconsin-Madison) etc.

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

❖ **Visiting Researcher, Oxford (September'2023- November'2023)**

Project: "Mössbauer Study on Iron-Catalyzed Asymmetric Multicomponent Cross-Coupling Strategies"

Supervisor: Prof. Michael Neidig, University of Oxford, United Kingdom

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 enantioselectivity

TEACHING AND MENTORING EXPERIENCE

❖ **Coordinator – Computational Chemistry Outreach Program (2022-Present)**

- ✓ Co-led *iCarbon* initiative, delivering weekly computational chemistry classes that increased equity in STEM by expanding research opportunities for underrepresented community college students.
- ✓ Designed and taught weekly virtual courses on DFT & molecular modeling while leading a team of 6 graduate mentors, delivering high-impact computational training to **15** undergraduates at Sacramento City College & Long Beach City College, strengthening their pathway into STEM research.

❖ **Graduate Mentor (2022-Present)**

- ✓ Supervised and mentored **6 trainees** (undergraduate & graduate) in independent computational and experimental research projects, encompassing organic synthesis, computational chemistry (DFT/MD), mechanistic analysis, and spectroscopy.

❖ **Graduate Teaching Assistant (2021-2023)**

- ✓ Delivered instruction & hands-on supervision in OChem labs, guiding students through synthesis, purification & spectroscopic techniques while reinforcing best practices in laboratory safety.

EDUCATION

PhD Chemistry, Texas A&M University (2021–Present) – GPA: 3.75

M.Sc. Chemistry, IIT Bombay (2021) – CPI: 9.69 | B.Sc. Chemistry, University of Delhi (2019) – CPI: 9.59

PUBLICATIONS

Co-author of **18** peer-reviewed articles (**2 First author, 8 second author**); 1 first author manuscript under review and 1 additional first author manuscript under preparation.

1. **Gogoi, A. R.**[#]; Mukherjee, P.[#]; Sinclair, B.[#]; Datta, A.; Briggs-Pritchard, J.; Guerrero, M.; Morehead, L.; Rao, P.; Neidig, M.; Gutierrez, O. Asymmetric Iron-Catalyzed Multicomponent Radical Dicarbofunctionalization of Vinyl Organoboron Compounds. *Under review*
2. **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.
3. **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*.
4. 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.
5. Elgindy, C.; **Gogoi, A. R.**; Rentería-Gómez, Á.; Park, B.; Das, D.; Obertone, C. E.; Dherange, B. D.; Gutierrez, O.; Levin, M. D. Mechanisms and Synthetic Applications of Cyclic, Nonstabilized Isodiazenes: Nitrogen-Atom Insertion into Pyrrolidines and Related Rearrangements. *J. Am. Chem. Soc.* **2025**, *147*, 28179–28188.
6. Peng, Q.; **Gogoi, A. R.**; Renteria-Gomez, A.; Gutierrez, O.; Scheidt, K. A., Visible Light-Induced Coupling of Carboxylic Acids with Alcohols and Amines, *Chem* **2023**.
7. Aguilera, M. C.; **Gogoi, A. R.**; Lee, W.; Liu, L.; Brennessel, W. W.; Gutierrez, O.; Neidig, M. L. Insight into Radical Initiation, Solvent Effects, and Biphenyl Production in Iron–Bisphosphine Cross-Couplings. *ACS Catal.* **2023**, *13*, 8987–8996.
8. Leong, D. W.; **Gogoi, A. R.**; Maity, T.; Lee, C.-I.; Bhuvanesh, N.; Gutierrez, O.; Ozerov, O. V. Abstraction of Hydride from Alkanes and Dihydrogen by the Perfluorotrityl Cation. *Angew. Chem. Int. Ed Engl.* **2025**, *64*, e202422190.
9. Das, M.; **Gogoi, A. R.**; Sunoj, R. B. Molecular Insights on Solvent Effects in Organic Reactions as Obtained through Computational Chemistry Tools. *J. Org. Chem.* **2022**, *87*, 1630–1640.
10. Youshaw, C. R.[#]; Yang, M.-H.[#]; **Gogoi, A. R.**; Rentería-Gómez, A.; Liu, L.; Morehead, L. M.; Gutierrez, O. Iron-Catalyzed Enantioselective Multicomponent Cross-Couplings of α-Boryl Radicals. *Org. Lett.* **2023**, *25*, 8320–8325.
11. Day, C. S.; **Gogoi, A. R.**[#]; Renteria-Gomez, A.[#]; Ton, S. J.[#]; Gutierrez, O.; Martin, R., Elucidating Electron-Transfer Events in Polypyridine Nickel Complexes for Reductive Coupling Reactions. *Nat. Catal.* **2023**, *6* , 244–253.
12. Kang, S.; Cen, W.; **Gogoi, A. R.**; Piña, J.; Suresh, A.; Ramirez, F.; Gutierrez, O.; Thomas, A. A. Mechanistically Driven Development of Kumada Catalyst-Transfer Polymerizations: A Rapid Injection NMR Study. *ACS Catal.* **2025**, 20773–20785.
13. Crockett, M.P.; Pina, J.; **Gogoi, A.R.**[#]; Lalisse, R. F.[#]; Nguyen, A.V.; Gutierrez, O.; Thomas, A. A. Breaking the tert-Butyllithium Contact Ion Pair: A Gateway to Alternate Selectivity in Lithiation Reactions, *J. Am. Chem. Soc.* **2023,** *145* , 10743–10755.
14. Wu, F.-P.; Lenz, M.; Suresh, A.[#]; **Gogoi, A. R.**[#]; Tyler, J. L.; Daniliuc, C. G.; Gutierrez, O.; Glorius, F. Nitrogen-to-Functionalized Carbon Atom Transmutation of Pyridine. *Chem. Sci.* **2024**, *15*, 15205–15211.
15. Zhu, J. L.; Schull, C. R.; Tam, A. T.; Rentería-Gómez, Á.; **Gogoi, A. R.**; Gutierrez, O.; Scheidt, K. A. Photoinduced Acylations via Azolium-Promoted Intermolecular Hydrogen Atom Transfer. *J. Am. Chem. Soc.* **2023**, *145*, 1535–1541.
16. Altundas, B.; Alwedi, E.; Song, Z.; **Gogoi, A. R.**; Dykstra, R.; Gutierrez, O.; Fleming, F. F. Dearomatization of Aromatic Asmic Isocyanides to Complex Cyclohexadienes. *Nat. Commun.* **2022**, *13*, 6444.
17. Thompson, R. R.; Figgins, M. T.; Wannipurage, D. C.; Renteria-Gomez, A.; **Gogoi, A. R.**; Telser, J.; Tierney, D. L.; Neben, M. C.; Demeshko, S.; Gutierrez, O.; Powers, D. C. P-P Coupling with and without Terminal Metal-Phosphorus Intermediates. *J. Am. Chem. Soc.* **2025**, *147*, 5350–5359.
18. Rentería-Gómez, A.; Lee, W.; Yin, S.; Davis, M.; **Gogoi, A. R.**; Gutierrez, O. General and Practical Route to Diverse 1-(Difluoro)Alkyl-3-Aryl Bicyclo[1.1.1]Pentanes Enabled by an Fe-Catalyzed Multicomponent Radical Cross-Coupling Reaction. *ACS Catal.* **2022**, *12*, 11547–11556.
19. Mandal, H.; Ogunyemi, O. J.; Nicholson, J. L.; Orr, M. E.; Lalisse, R. F.; Rentería-Gómez, Á.; **Gogoi, A. R.**; Gutierrez, O.; Michaudel, Q.; Goodson, T., 3rd. Linear and Nonlinear Optical Properties of All-Cis and All-Trans Poly(p-Phenylenevinylene). *J. Phys. Chem. C Nanomater. Interfaces* **2024**, *128*, 2518–2528.

full list of manuscripts under review or preparation is available: https://achyutrgogoi.github.io

LEADERSHIP & SERVICE

- Recipient of the **Sharon Dabney Memorial Scholarship** for excellence in research and departmental leadership at Texas A&M University.
- **Secretary** at Phi Lambda Upsilon: The Honorary Chemical Society of Texas A&M University, 2024.
- Physical Chemistry Division Representative at Chemistry Student Safety Committee (CSSC) Board 2024.
- Graduate Student Member: American Chemical Society, 2024.

SELECTED TALKS & PRESENTATIONS

Delivered more than 10 scientific talks aimed at diverse audiences, translating complex mechanisms and computational models into accessible visuals for students and faculty.

- SACNAS Diversity in Science Symposium 2023 – Poster Award (**3rd Place**)
- ACS-Division of Organic Chemistry Graduate Research Symposium 2025, San Diego – Oral Presentation titled "*Synergizing Computation and Experiments for Sustainable Reaction Design".*
- ACS Fall 2024, Denver – Oral Presentation titled **"***Mechanistic Insight Guided Rational Design of Iron-Catalyzed Asymmetric Multicomponent Cross-Coupling Strategies***"**.
- Gordon Research Conference (Physical Organic Chemistry) 2023 – Poster Presentation titled **"***Fe-Catalyzed Asymmetric Multicomponent Cross-Coupling Reactions: Scope and Mechanistic Insights***".**
- Catalysis Innovation Consortium (CIC) System Wide Meeting 2025, Emory University - Virtual oral talk titled "*Synergizing Computation and Experiments for Sustainable Reaction Design*".
- Theoretical and Physical Organic Chemistry (TPOC) Monthly Meeting 2023, University of Houston and UC Davis - Virtual oral talk titled "*Harnessing the symbiotic potential of computation and experiment for sustainable iron catalysis*".
- Catalysis Innovation Consortium (CIC) Annual Meeting 2024, Emory University - Poster titled "*Mechanistic Insight Guided Rational Design of Iron-Catalyzed Asymmetric Multicomponent Cross-Coupling Strategies*".
- Welch Conference 2024**,** Houston **-** Poster titled "*Mechanistic Insight Guided Rational Design of Iron-Catalyzed Asymmetric Multicomponent Cross-Coupling Strategies*".
- Cotton Medal Conference 2023 and 2024**,** Texas A&M University **-** Poster titled "*Mechanistic Insight Guided Rational Design of Iron-Catalyzed Asymmetric Multicomponent Cross-Coupling Strategies*".
- Houk Research Conference 2022, UCLA - Poster titled "*Computational Investigation into Electron Transfer Events in Polypyridine Ligated Nickel Complexes*".

PROFESSIONAL MEMBERSHIP

ACS Member | CIC (Catalysis Innovation Consortium) Student Ambassador | Recruitment & Open House Team Member in Texas A&M University Chemistry Department.

CORE SKILLS

Computational Chemistry (DFT & MD) | Cross-functional Collaboration

Organic Synthesis: Asymmetric Catalysis | Mössbauer Spectroscopy | HTE | Coding (C++, Python)

Curriculum Design | Creating problem sets & rubrics | Student mentoring & evaluation

TECHNICAL SKILLS

Instruments: Mössbauer Spectrometer, NMR, RI-NMR, FT-IR, UV-Vis, Spectrofluorometer, Polarimeter

Software: Gaussian, ORCA, GAMESS, Avogadro, AutoCAD, PyMOL

Programming: Python, C++, Arduino, FORTRAN, MySQL