

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 with direct relevance to pharmaceutical R&D. Passionate about applying computational chemistry and mechanistic insight to accelerate data-rich experimentation and drug discovery.

RESEARCH EXPERIENCE

❖ Visiting Graduate Researcher (June'2025- Present)

Project Title: **Development of Iron Catalyzed Asymmetric Reductive Cross Electrophile Coupling using High Throughput Experimentation (HTE) and DFT**

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

- ✓ Leading the development of iron-catalyzed asymmetric reductive cross-electrophile coupling reactions through high-throughput experimentation and data-driven reaction design.

❖ PhD Research (August'2021-Present)

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

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

- ✓ Developed sustainable **asymmetric** multicomponent iron-catalyzed cross-coupling strategy for the **enantioselective synthesis** of chiral boronic esters (**~98% e.e.**); elucidated detailed mechanistic pathways through integrated **DFT** modeling and **Mössbauer spectroscopic** analysis.

Project 2 Title: **Harnessing the Symbiotic Potential of Computation & Experiment in Elucidation of Reaction Mechanisms.**

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

- ✓ Collaborated with groups across the globe (ICIQ, UChicago, Northwestern, Oxford, UW-Madison, NUS, University of Münster etc.) using **DFT & Molecular Dynamics** to investigate mechanisms across iron, nickel, palladium and metal-free catalytic transformations leading to **18+ high impact publications**.

❖ Visiting Graduate Researcher (September'2023- November'2023)

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

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

- ✓ Conducted in-depth **Mössbauer spectroscopy** experiments to identify & characterize the active stereodetermining iron species, contributing to a deeper understanding of reaction mechanisms for the development of more effective iron based catalytic strategies.

SELECTED PUBLICATIONS

Co-author of **18** peer-reviewed articles (**2 First author, 8 second author**), including in Nature Catalysis, Nature Communications, JACS, ACS Catalysis, Chem, Angew. Chem., etc.; **2 more 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.
4. 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**.

Full list available at: <https://achyutrgogoi.github.io>

CORE SKILLS

Computational Chemistry (DFT & MD) Cross-functional Collaboration	★★★★★ 5.0
Organic Synthesis: Asymmetric Catalysis Reaction Mechanism Elucidation	★★★★★ 5.0
Mössbauer Spectroscopy HTE Inorganic Synthesis Coding (Python, C++, Arduino)	★★★★★ 4.5

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

TECHNICAL SKILLS

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

Software: Gaussian, ORCA, GAMESS, Avogadro, AutoCAD

SELECTED TALKS & PRESENTATIONS

- SACNAS Diversity in Science Symposium 2023 – Poster Award (**3rd Place**)
- ACS-Division of Organic Chemistry Graduate Research Symposium 2025, San Diego – Oral Presentation
- ACS Fall 2024, Denver – Oral Presentation
- Gordon Research Conference (Physical Organic Chemistry) 2023 – Poster Presentation
- Catalysis Innovation Consortium Systemwide Meeting 2025 – Virtual Oral Talk

LEADERSHIP & SERVICE

- Recipient of the **Sharon Dabney Memorial Scholarship** for excellence in research and departmental leadership at Texas A&M University
- **Secretary**, Phi Lambda Upsilon (PLU), Texas A&M University Chemistry Honor Society
- Co-led the iCarbon initiative by designing & **delivering weekly computational chemistry workshops** (DFT, molecular modeling), expanding equitable access to STEM research for **15+** students from Sacramento City College and Long Beach City College
- Chemistry Student **Safety Committee member** at Texas A&M, Chemistry Department

ADDITIONAL INVOLVEMENT

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