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 **17+ high-impact publications** and international collaborative research with leading groups across **10+ universities**. *Expertise in 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

❖ **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 **asymmetric** multicomponent iron-catalyzed cross-coupling strategies for the **enantioselective synthesis** of chiral boronic esters **(>94% e.e.**); elucidated detailed mechanistic pathways through integrated **DFT** modeling and **Mössbauer spectroscopic** analysis.
  - ✓ *Manuscripts under preparation*

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

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

- ✓ Utilized advanced tools (**DFT & Molecular Dynamics**) to investigate mechanisms across iron, nickel, and rhodium and metal-free catalytic transformations leading to high impact publications.
- ✓ Collaborated with groups across the globe (ICIQ, UChicago, Northwestern, UW–Madison, Oxford) resulting in **17+ high impact publications**.

❖ **Visiting 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 investigate iron speciation in asymmetric iron-catalyzed multicomponent cross-coupling reactions.
- ✓ Identified and characterized the stereodetermining active iron species, contributing to a deeper understanding of reaction mechanisms for the development of more effective catalytic strategies.
  - ✓ *Manuscripts under preparation*

SELECTED PUBLICATIONS

Co-author of **17** peer-reviewed articles (**2 First author, 8 second author**), including in Nature Catalysis, Nature Communications, JACS, ACS Catalysis, Chem, Angew. Chem., Org. Lett. etc. ; 2 more first author manuscripts under preparation.

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   ★★★★⯪ 4.5

Mössbauer Spectroscopy | HTE | Inorganic Synthesis | Coding (Python, C++)   ★★★★☆ 4

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

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

Software: Gaussian, ORCA, GAMESS, Avogadro, AutoCAD

SELECTED TALKS & PRESENTATIONS

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

LEADERSHIP & SERVICE

- Secretary, Phi Lambda Upsilon (PLU), Texas A&M University Chemistry Honor Society
- Recipient of the **Sharon Dabney Memorial Scholarship** for excellence in research and departmental leadership at Texas A&M University.
- Co-led iCarbon – An outreach program to teach computational chemistry to underrepresented students in community colleges (Sacramento Community College and Los Angelese 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.