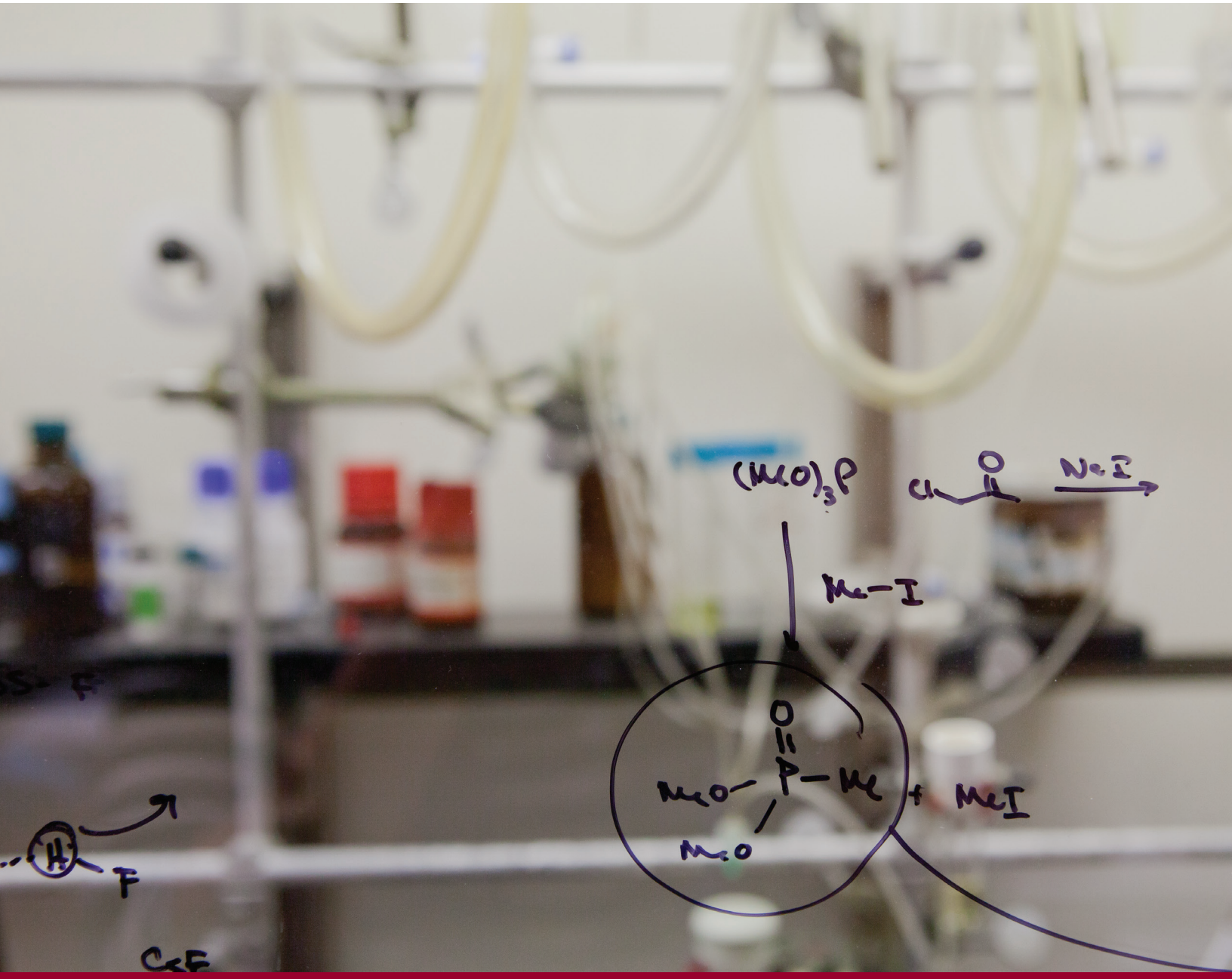
BOSTON COLLEGE

Morrissey College of Arts and Sciences



GRADUATE PROGRAM

Chemistry

A MESSAGE FROM THE CHEMISTRY FACULTY AT BOSTON COLLEGE

Welcome to the Department of Chemistry at Boston College. Our department is a dynamic research community comprised of nearly 200 scientists studying all phases of contemporary chemical science, including many interdisciplinary areas interfacing with the fields of biology, medicine, physics, and materials science. More than 100 graduate students, 40 undergraduate majors, and 25 postdoctoral fellows work hand in hand with approximately 20 internationally recognized and acclaimed faculty members advancing the frontiers of chemistry. In addition, we annually host a diverse seminar series that brings outstanding visiting scientists from around the world to campus for formal and informal interactions with all members of the department.

Recent achievements of the scientists in the Department of Chemistry reflect our exciting research culture. In the last year, more than 70 research papers were published by BC chemists in internationally recognized journals, including *Nature, Science, Nature Chemistry, Nature Chemical Biology, Journal of the American Chemical Society,* and *Angewandte Chemie*; the overwhelming majority of these papers were co-authored by our graduate students. Each year, we celebrate the accomplishments of our students with a Graduate Student Research Symposium, a daylong event featuring seminars and poster presentations by our graduate student colleagues.

Many of our graduate students have obtained prestigious fellowships, including those sponsored by the American Chemical Society, the Department of Education, the National Institutes of Health, the National Science Foundation, the Department of Energy, NASA, and the pharmaceutical industry. In addition, graduates of the department have gone on to assume positions of scientific leadership in private industry as well as in some of the finest academic institutions in the world.

For a genuine appreciation of the exciting atmosphere of the department and the outstanding facilities that provide the setting for our research, we strongly encourage you to view our website or plan a campus visit. We would be happy to arrange individual meetings with faculty and students so that you can get a firsthand sense of the vibrant scientific environment of our department. For more information, please e-mail us at chemadmissions@bc.edu.

CONTENTS

PROGRAM OVERVIEW

Ph.D. Program

Graduate Curriculum

The curriculum is designed to provide students with the skills necessary to succeed as independent researchers, stimulate intellectual exchange among students and faculty members, and develop oral and written communication skills.

First-year course requirements provide students with a breadth of knowledge in the traditional fields: organic, chemical biology, physical chemistry, and inorganic chemistry. While a specific number of credits is not required for the Ph.D., students are encouraged to pursue a program of studies—with the approval of their advisor—that is consistent with their individual educational goals.

Curriculum Outline:

Year 1	Coursework
Year 2	Qualifying Exam
Year 3	Student Department Seminar
Year 4	Original Proposal

Selection of a Research Advisor

During the first semester of graduate studies, students meet with faculty members and advanced graduate students to explore the dissertation project opportunities available in various research groups. The Graduate Student Research Symposium, held in October, showcases the research of our graduate students in a daylong event that consists of oral and poster presentations. The symposium is an excellent opportunity for new graduate students to learn more about research activities in the department. By the end of the first semester, most students have selected a research advisor and identified a potential dissertation project that they will begin investigating in the second semester.

Teaching Requirements

Some teaching or equivalent educational experience is required. This requirement may be satisfied by at least one year of service as a teaching assistant or by other suitable teaching duties. Arrangements are made with each student for a teaching program best suited to their overall program of study. Waivers of teaching requirements may be granted under special circumstances with the approval of the Department of Chemistry.

Comprehensive Examinations

At the end of the second year, Ph.D. students must pass an oral candidacy exam that focuses on material from their own research specialty and other related areas. Members of the student's dissertation committee (usually selected at the beginning of the second year) comprise their thesis committee.

Student Department Seminar and Original Proposal

During the third year, Ph.D. students present a seminar to the department summarizing their project goals and achievements to date. At the end of the fourth year, Ph.D. students submit and defend an original research proposal on a project outside of their direct research focus. Student's performance at both the seminar and proposal is evaluated by their thesis committee.

Dissertation and Defense

The Ph.D. requires completion of a written dissertation based upon original research performed by the student, either experimental or theoretical. For the Ph.D. candidate, a research project requiring three to four years of sustained effort will usually begin after the first year of study. An oral defense of the dissertation before a faculty committee completes the degree.

FACULTY PROFILES

JUNWEI LUCAS BAO

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RESEARCH INTERESTS

We develop theories and computer algorithms to reveal the underlying physical principles that govern the complex kinetics and dynamical behaviors of a variety of intriguing chemical systems, ranging from gas-phase collisions to interfacial and condensed-phase reactions. We are interested in understanding the electronic structure of reactive intermediates, the physical aspect of organic and inorganic catalysts, the reaction mechanisms, and the detailed kinetics of clean-energy-driven catalysis, including electrocatalysis and photocatalysis. We are curious about how reliable our theoretical tools can be for predicting the intricate catalytic kinetic information, such as activation energy, kinetic isotope effect, and selectivity. More importantly, if our current theoretical tools are not adequate, we strive to improve them or create new methods. We also embrace the power of data science and machine learning in some aspects of our research, (e.g., materials design, quantum chemistry), but with a focus centered on the underlying physics. Another topic in our group is investigating the interaction between chemistry and our environment. We aim to establish reliable and comprehensive atmospheric chemical kinetics models for studying the fate and distributions of important trace gases and reactive intermediates in the troposphere. Interdisciplinary and innovative, our team brings together quantum mechanics, statistical thermodynamics, solid-state physics, and other branches of physics and applied mathematics to tackle the challenges that arise from the intrinsic complexities of chemistry.

SELECTED PUBLICATIONS

- "Physical Prior Mean Function-Driven Gaussian Processes Search for Minimum-Energy Reaction Path with Climbing-Image Nudged Elastic Band: A General Method for Gas-Phase, Interfacial, and Bulk-Phase Reactions." Teng, C.; Wang, Y.; Bao J.L. *Journal of Chemical Theory and Computation*. 2024, 20(10), 4308-24.
- "Dual-Level Training of Gaussian Processes With Physically Inspired Priors for Geometry Optimizations." Teng, C.; Wang, Y.; Huang, D.; Martin, K.; Tristan, J.-B.; Bao J.L. *Journal of Chemical Theory and Computation*. 2022, 18, 5739-54.
- "Plasmon-Driven Carbon-Fluorine (C(sp3)-F) Bond Activation with Mechanistic Insights into Hot-Carrier-Mediated Pathways." Robatjazi, H.; Bao, J.L. et al. *Nature Catalysis*. 2020, 3, 564-73.
- "Rationalizing the Hot-Carrier-Mediated Reaction Mechanisms and Kinetics for Ammonia Decomposition on Ruthenium-Doped Copper Nanoparticles." Bao, J.L.; Carter, E.A. *Journal of the American Chemical Society*. 2019, 141, 13320-23.
- "Rapid Unimolecular Reaction of Stabilized Criegee Intermediates and Implications for Atmospheric Chemistry." Long, B.; Bao, J.L.; Truhlar, D.G. *Nature Communications*. 2019, 10, 2003.
- "Self-Interaction Error in Density Functional Theory: An Appraisal." Bao, J.L.; Gagliardi, L.; Truhlar, D.G. *The Journal of Physical Chemistry Letters*. 2018, 9, 2353-58.
- "Variational Transition State Theory: Theoretical Framework and Recent Developments." Bao, J.L.; Truhlar, D.G. *Chemical Society Review*. 2017, 46, 7548-96.
- "Predicting Bond Dissociation Energies of Transition Metal Compounds by Multiconfiguration Pair-Density Functional Theory and Second-Order Perturbation Theory Based on Correlated Participating Orbitals and Separated Pairs." Bao, J.L; Odoh, S.O.; Gagliardi, L.; Truhlar, D.G. *Journal of Chemical Theory and Computation*. 2017, 13, 616-26.
- "Barrierless Association of CF_2 and Dissociation of C_2F_4 by Variational Transition-State Theory and System-Specific Quantum Rice–Ramsperger–Kassel Theory." Bao, J.L.; Zhang, X.; Truhlar, D.G. *Proceedings of the National Academy of Sciences U.S.A.* 2016, 113, 13606-11.

ABHISHEK CHATTERJEE

Professor

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RESEARCH INTERESTS

The central theme of our research is engineering biology for developing next-generation bio-therapeutics, as well as novel tools to probe complex biological questions. We take an interdisciplinary approach that combines elements from chemistry, biology, and engineering. One particular focus of our group is a technology that enables precise incorporation of novel noncanonical amino acids (ncAAs) into proteins expressed in living cells. We pursue the following aims to expand the scope of this technology and use it for various applications: 1) Engineer new platforms to expand the structural diversity of ncAAs that are accessible using this technology; 2) Develop novel directed evolution approaches to engineer cellular translation for improving the efficiency of ncAA incorporation; 3) Develop new bioorthogonal

conjugation chemistries to enable site-specific protein labeling at multiple distinct sites; 4) Create tnext-generation biotherapeutics, such as therapeutic protein conjugates for immuno-oncology, as well as engineered adeno-associated virus conjugates for human gene therapy; 5) Model various post-translational modifications of human proteins to understand their roles in our biology; and 6) Probe proteomic changes that underlie complex biological processes such as the development of antibiotic resistance in pathogenic bacteria.

SELECTED PUBLICATIONS

- "Electrochemical Labelling of Hydroxyindoles with Chemoselectivity for Site-Specific Protein Bioconjugation." Loynd, C.; Singha Roy, S.J.; Ovalle, V.J.; Canarelli, S.E.; Mondal, A.; Jewel, D.; Ficaretta, E.D.; Weerapana, E.; Chatterjee, A. *Nature Chemistry*. 2024, 16(3), 389-97.
- "An Efficient Opal-Suppressor Tryptophanyl Pair Creates New Routes for Simultaneously Incorporating up to Three Distinct Noncanonical Amino Acids into Proteins in Mammalian Cells." Osgood, A.O.; Zheng, Y.; Roy, S.J.S.; Biris, N.; Hussain, M.; Loynd, C.; Jewel, D.; Italia, J.S.; Chatterjee, A. *Angewandte Chemie International Edition*. 2023, 62(19), 32022219269.
- "Virus-assisted Directed Evolution of Enhanced Suppressor tRNAs in Mammalian Cells." Jewel, D.; Keleman, R.E.; Huang, R.L.; Zhu, Z.; Sundaresh, B.; Cao, X.; Malley, K.; Huang, Z.; Pasha, M.; Anthony, J.; van Opijnen, T.; Chatterjee, A. *Nature Methods*. 2023, 20, 95-103.
- "A Facile Platform to Engineer Escherichia coli Tyrosyl-tRNA Synthetase Adds New Chemistries to the Eukaryotic Genetic Code, Including a Phosphotyrosine Mimic." Grasso, K.T.; Roy, S.J.S.; Osgood, A.O.; Yeo, M.J.R.; Soni, C.; Hillebrand, C.M.; Ficaretta, E.D.; Chatterjee, A. *ACS Central Science*. 2022, 8(4), 483-92.
- "Genetically Encoded Protein Sulfation in Mammalian Cells." Italia, J.S.; Peeler, J.C.; Hillenbrand, C.M.; Latour, C.; Weerapana, W.; Chatterjee; A. *Nature Chemical Biology*. 2020, 16, 379-82.
- "Mutually Orthogonal Nonsense-suppression Systems and Conjugation Chemistries for Precise Protein Labeling at Up to Three Distinct Sites." Italia, J.S.; Addy, P.S.; Erickson, S.B.; Peeler, J.C.; Weerapana, E.; Chatterjee, A. *Journal of the American Chemical Society*. 2019, 141, 6204-12.
- "An Orthogonalized Platform for Genetic Code Expansion in Both Bacteria and Eukaryotes." Italia, J.S.; Addy, P.S.; Wrobel, C.J.J.; Crawford, L.A.; Lajoie, M.J.; Zheng, Y.; Chatterjee, A. *Nature Chemical Biology*. 2017, 13(4), 446-50.

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RESEARCH INTERESTS

An overarching goal of the Gao group research is to understand the chemical basis of important molecular interactions underlying normal physiology and disease. We take a synthetic approach toward this goal; namely, we design and synthesize molecular probes to interrogate the role of important proteins and lipids pertinent to antibiotic resistance and cancer. A major innovation of our work involves the design and synthesis of "chemical warheads" to enable novel modes of binding and inhibition of biomolecules. For example, our recent work has showcased the potential of probe/inhibitor design using pi-pi interactions as well as dynamic covalent binding mechanisms, which nicely complement canonical mechanisms like hydrogen bonds and electrostatic interactions. These innovative approaches are deeply rooted in organic chemistry; more specifically, a deep understanding of physical organic chemistry and chemoselective reactions. Importantly, we have developed a peptide-based molecular discovery platform in which novel peptide libraries are constructed to incorporate chemical warheads of our design. Screening of such peptide libraries allows facile discovery of novel molecular probes and inhibitors for various targets that have challenged traditional small molecule drugs.

SELECTED PUBLICATIONS

- "Lysine-Targeting Reversible Covalent Inhibitors with Long Residence Time." Reja, R.M.; Wang, W.; Lyu, Y.; Haeffner, F.; Gao, J. *Journal of the American Chemical Society*. 2022, 144, 1152-57.
- "Versatile Conjugation Chemistries of ortho-Boronyl Aryl Ketones and Aldehydes." Cambray, S.; Gao, J. *Accounts of Chemical Research*. 2018, 51, 2198-206.
- "Phage Display of Dynamic Covalent Binding Motifs Enables Facile Development of Targeted Antibiotics." McCarthy, K.A.; Kelly, M.A.; Li, K.; Cambray, A.; Hosseini, A.S.; van Opijnen, T.; Gao, J. *Journal of the American Chemical Society*. 2018, 140, 6137-45.
- "Fast Diazaborine Formation of Semicarbazide Enables Facile Labeling of Bacterial Pathogens." Bandyopadhyay, A.; Cambray, S.; Gao, J. *Journal of the American Chemical Society*. 2017, 139, 871-78.
- "Targeting Biomolecules with Reversible Covalent Chemistry." Bandyopadhyay, A.; Gao, J. *Current Opinion in Chemical Biology*. 2016, 34, 110-16.

FACULTY PROFILES

✣ "Iminoboronate-Based Peptide Cyclization That Responds to pH, Oxidation, and Small Molecule Modulators." Bandyopadhyay, A.; Gao, J. *Journal of the American Chemical Society*. 2017, 139, 871-78.
✣ "Targeting Bacteria via Iminoboronate Chemistry of Amine-Presenting Lipids." Bandyopadhyay, A.; McCarthy, K.A.; Kelly, M.A.; Gao, J. *Nature Communications*. 2015, 6, 6561.

ALEXIS GRIMAUD

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RESEARCH INTERESTS

Our research lies at the frontier between materials science for electrode design and physical chemistry of liquid electrolytes. We apply these principles to understand and develop efficient electrochemical energy storage and conversion devices with an emphasis on secondary (rechargeable) batteries, water electrolyzers, and the electrosynthesis of commodity chemicals. Our research relies on a solid-state chemist approach with the control of bulk redox and conduction (ionic and electronic) properties of transition metal-based materials for Li-ion batteries. Recognizing that bulk intercalation opens broad scientific opportunities beyond the simple study of novel Li-ion battery electrode materials, we investigate intercalation processes for fine-tuning of electronic properties of materials. Furthermore, we seek to illuminate the influence of electrolyte on the charge transfer kinetics at solid/liquid interfaces, ubiquitous to electrochemical systems, and liquid/liquid interfaces relevant to novel battery chemistries. To this end, we foster new strategies to control the liquid water environment at the nanoscale. Our approach allows drawing a structure/reactivity for water at electrochemical interfaces, which we apply to the electrochemical synthesis of more complex organic molecules.

SELECTED PUBLICATIONS

✣ "Direct Imaging of Micrometer Thick Interfaces in Salt-Salt Aqueous Biphasic Systems." Degoulange, D.; Pandya, R.; Deschamps, M.; Sikiba, D.A.; Gallant, B.M.; Gigan, S.; de Aguiar, H.B.; Grimaud, A. *Proceedings of the National Academy of Science*. 2023,120(17), e2220662120.
✣ "Design of Workflows for Cross-talk Detection and Lifetime Deviation Onset in Li-ion Batteries." Meunier, V.; Leal de Souza, M.; Morcrette, M.; Grimaud, A. *Joule*. 2023, 7, 42-56.
✣ "Controlling the Hydrophilicity of the Electrochemical Interface to Modulate the Oxygen-atom Transfer in Electrocatalytic Reactions." Dorchies, F.; Serva, A.; Crevel, D.; De Freitas, J.; Kostopoulos, N.; Robert, M.; Sel, O.; Salanne, M.; Grimaud, A. *Journal of the American Chemistry Society*. 2022, 144, 22734-46.
✣ "Three-dimensional Operando Optical Imaging of Particle and Electrolyte Heterogeneities Inside Li-ion Batteries." Pandya, R.; Valzania, L.; Dorchies, F.; Xia, F.; Mc Hugh, J.; Mathieson, A.; Tan, H.J.; Parta, T.G.; Godeffroy, L.; Mazloomian, K.; Miller, T.S.; Kanoufi, F.; De Volder, M.; Tarascon, J.-M.; Gigan, S.; de Aguiar, H.; Grimaud, A. *Nature Nanotechnology*. 2023, 18, 1185-94.

AMIR HOVEYDA

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RESEARCH INTERESTS

Making it easier for scientists to access organic molecules that they believe might have a special function is what we care about most. We are less interested in structure or selectivity for its own sake. Our main objective is either to introduce new functional molecules, such as catalysts, or develop catalytic strategies that will facilitate generating them. In regard to catalyst discovery, the design and development of Mo, W, or Ru complexes that promote stereocontrolled olefin metathesis reactions that furnish trisubstituted alkenes has been one area of interest. We have begun to tackle the still-more-challenging task of finding catalysts that are effective at delivering tetrasubstituted olefins in either stereoisomeric form, which will be of considerable utility in drug discovery and development. A more recent area of activity entails introducing catalysts and catalytic approaches that can be used to synthesize efficiently as well as enantio- and diastereodivergently. Our aim is to accomplish this by a shared network of reactions, not only a natural product but also the corresponding unnatural and precisely altered skeletal analogs. We recently completed a project where we designed a catalytic multicomponent enantioselective reaction that was used to access a rare polycyclic indole alkaloid as well as various one-two methylene expanded, contracted and distorted frameworks. This allowed us to discover that a doubly expanded framework is cytotoxic against the four cancer cells screened (3mM). No other compound in the collection, including the mildly anti-malarial natural product, showed any cytotoxicity. Equally important to us are computational studies, including

molecular dynamics and AI-accelerated docking studies, which we perform through close collaboration with the appropriate experts. Projects involving the design and development of catalysts and catalytic strategies for late stage skeletal alterations of complex and readily bioactive natural products is another exciting new area for us. We seek new molecular vistas means that we are most keen to introduce new click reactions that are orthogonal to the existing alternatives (CuAAC and SuFEx, for example) and deliver modifiable, distinguishable, and clippable linkages. We approach chemical synthesis conceptually.

SELECTED PUBLICATIONS

- "A Catalytic Process Enables Efficient and Programmable Access to Precisely Altered Indole Alkaloid Scaffolds." Huang, Y.; Li, X.; Mai, B.K.; Tonogai, E.J.; Smith, A.J.; Hergenrother, P.J.; Liu, P.; Hoveyda, A.H. *Nature Chemistry*. 2024, 16, 1003-14.
- "Click Processes Orthogonal to Cuaac and Sufex Forge Selectively Modifiable Fluorescent Linkers." Paioti, P.H.S.; Lounsbury, K.E.; Romiti, F.; Formica, M.; Bauer, V.; Zandonella, C.; Hackey, M.E.; Del Pozo, J.; Hoveyda, A.H. *Nature Chemistry*. 2024, 16, 426-36.
- "Diastereo- and Enantioselective Synthesis of Compounds With a Trifluoromethyl- and Fluoro-Substituted Carbon Center." Xu, X.; Del Pozo, J.; Romiti, F.; Fu, Y.; Mai, B.K.; Morrison, R.J.; Lee, K.; Hu, S.; Koh, M.J.; Lee, J.; Li, X.; Liu, P.; Hoveyda, A.H. *Nature Chemistry*. 2022, 14, 1459-69.
- "Z, E- and -Trisubstituted Macrocyclic Alkenes for Natural Product Synthesis and Skeletal Editing." Mu, Y.; Hartrampf, F.W.W.; Yu, E.C.; Lounsbury, K.E.; Schrock, R.R.; Romiti, F.; Hoveyda, A.H. *Nature Chemistry*. 2022, 14, 640-49.
- "Stereodefined Alkenes With a Fluoro-Chloro Terminus as a Uniquely Enabling Class of Compounds." Liu, Q.; Mu, Y.; Koengeter, T.; Schrock, R.R.; Hoveyda, A.H. *Nature Chemistry*. 2022, 14, 463-73.
- "Delayed Catalyst Function Enables Direct Enantioselective Conversion of nitriles to NH2-amines." Zhang, S.; del Pozo, J.; Romiti, F.; Mu, Y.; Torker, S.; Hoveyda, A.H. *Science*. 2019, 364, 45-51.
- "Mechanism-based Enhancement of Scope and Enantioselectvity for Reations Involving a Copper-Substituted Stereogenic Carbon Centre." Lee, J.; Radomkit, S.; Torker, S.; del Pozo, J.; Hoveyda, A.H. *Nature Chemistry*. 2018, 10, 99-108.

JIER HUANG

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RESEARCH INTERESTS

Research in the Huang group is centered on developing cutting-edge materials for applications in solar energy conversion. This effort involves the design, synthesis, and spectroscopic characterization of hybrid porous crystalline and semiconducting materials, with our aim to correlate the structure of these materials with their photophysical and photochemical properties. Currently investigated materials include covalent organic frameworks (COFs), zeolitic imidazolate frameworks (ZIFs), metal organic frameworks (MOFs), and semiconductor nanocrystals. Using a set of complimentary spectroscopic techniques, including optical transient absorption (OTA), X-ray transient absorption (XTA), and in situ X-ray absorption spectroscopy (XAS), we seek to probe the unknown and underexplored photophysical properties and gain a better understanding of the property/function relationships of these materials.

SELECTED PUBLICATIONS

- "Modulating the Primary and Secondary Coordination Spheres of Single Ni(II) Sites in Metal-Organic Frameworks for Boosting Photocatalysis." Yang, G.; Wang, D.; Wang, Y.; Hu, W.; Hu, S.; Jiang, J.; Huang, J.; Jiang, H. *Journal of the American Chemical Society*. 2024, 146, 10798-805.
- "Control Over Charge Separation by Imine Structural Isomerization in Covalent Organic Frameworks with Implications on CO2 Photoreduction." Streater, D.H.; Kennehan, E.R., Wang, D.; Fiankor, C.; Chen, L.; Yang, C.; Li, B.; Liu, D.; Ibrahim, F.; Hermans, I.; Kohlstedt, K.L.; Luo, L.; Zhang, J.; Huang, J. *Journal of the American Chemical Society*. 2024, 146, 4489-99.
- "Dominant Role of Hole Transport Pathway in Achieving Record High Photoconductivity in Two-Dimensional Metal—Organic Frameworks." Wang, D.; Ostresh, S.; Streater, D.; He, P.; Nyakuchena, J.; Ma, Q.; Zhang, X.; Neu, J.; Brudvig, G.W.; Huang, J. *Angewandte Chemie International Edition*, 2023, e202309505.
- "Symmetry-Guided Synthesis of N,N'-Bicarbazole and Porphyrin-Based Mixed-Ligand Metal-Organic Frameworks: Light Harvesting and Energy Transfer." Fiankor, C.; Nyakuchena, J.; Khoo, R.; Zhang, X.; Hu, Y.; Yang, S.; Huang, J.; Zhang, J. *Journal of the American Chemical Society*. 2021, 143, 20411-18.

FACULTY PROFILES

- "Conjugation and Aggregation Directed Design of Covalent Organic Frameworks as White Light-Emitting Diode." Yang, S.; Streater, D.; Fiankor, C.; Zhang, J.; Huang, J. *Journal of the American Chemical Society*. 2021, 143, 1061-68.
- "Direct Evidence of Photoinduced Charge Transport Mechanism in 2D Conductive Metal Organic Frameworks." Nyakuchena, J.; Ostresh, S.; Streater, D.; Pattengale, B.; Fiankor, C.; Hu, W.; Kinigstein, E.D.; Zhang, J.; Zhang, X.; Schmuttenmaer, C.A.; Huang, J. *Journal of the American Chemical Society*. 2020, 120, 21050-58.
- "Dynamic Evolution and Reversibility of Single-atom Ni(II) . Active Site in 1T-MoS2 Electrocatalysts for Hydrogen Evolution." Pattengale, B.; Huang, Y.; Yan, X.; Yang, S.; Younan, S.; Hu, W.; Li, Z.; Lee, S.; Pan, X.; Gu, J.; Huang, J. *Nature Communications*, 2020, 11, 4114.
- "Tuning Internal Strain in Metal-Organic Frameworks via Vapor Phase Infiltration for CO2 Reduction." Yang, F.; Hu, W.; Patrick, M.; Cooksy, A.L.; Aguiar, J.A.; Fang, C.; Zhou Y., Meng, Y.S.; Huang, J.; Gu, J. *Angewandte Chemie International Edition*. 2020, 59, 2-11.
- "2D Covalent Organic Frameworks as Intrinsic Photocatalysts for Visible Light Driven CO 2 Reduction." Yang, S.; Hu, W.; Zhang, X.; He, P.; Pattengale, B.; Liu, C.; Cendejas, M.; Hermes, I.; Zhang, X.; Zhang, J.; Huang, J. *Journal of the American Chemical Society*. 2018, 140, 14614-18.
- "Donor-Acceptor Fluorophores for Energy Transfer Mediated Photocatalysis." Lu, J.; Pattengale, B.; Liu, Q.; Yang, S.; Shi, W.; Li, S.; Huang, J.; Zhang, J. *Journal of the American Chemical Society*. 2018, 140, 13719-25.
- "Direct Observation of Node-to-Node Communication in Zeolitic Imidazolate Frameworks." Pattengale, B.; SantaLucia, D.; Yang, S.; Hu, W.; Liu, C.; Zhang, X.; Berry, J.; Huang, J. Journal of the American Chemical Society. 2018, 140, 11573-76.
- "Exceptionally Long-Lived Charge Separated State in Zeolitic Imidazolate Framework: Implication for Photocatalytic Applications." Pattengale, B.; Yang, S.; Ludwig, J.; Huang, Z.; Zhang, X.; Huang, J. *Journal of the American Chemical Society*. 2016, 138, 8072-75.

SHIH-YUAN LIU

Professor

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RESEARCH INTERESTS

We are interested in the development of boron (B)-nitrogen (N)-containing heterocycles, specifically azaborines. These are structures resulting from the replacement of two carbon atoms in benzene with a boron and a nitrogen atom. Azaborines are isosteres of the important family of benzenoid compounds/arenes. They closely match the size and shape of ordinary benzene rings, and they still enjoy considerable aromatic stabilization, but most of their other physical, chemical, and spectroscopic properties are significantly altered. We aim to exploit the unique properties of azaborines and investigate their potential as arene surrogates in materials and biomedical research. Our approach combines the broad utility of arenes with the unique elemental features of boron. Areas of exploration include organic synthesis, catalysis, energy storage, optoelectronic materials, and drug discovery. The development of azaborines has the potential of changing the way chemists think about creating molecular diversity and new functions, namely through BN/CC isosterism.

SELECTED PUBLICATIONS

- "A BN-Doped Cycloparaphenylene Debuts." Chen, M.; Unikela, K.S.; Ramalakshmi, R.; Li, B.; Darrigan, C.; Chrostowska, A.; Liu, S.-Y. *Angewandte Chemie International Edition*. 2021, 60, 1556-60.
- "Pd-Senphos Catalyzed Trans-Selective Cyanoboration of 1,3-Enynes." Zhang, Y.; Li, B.; Liu, S.-Y. *Angewandte Chemie International Edition*. 2020, 59, 15928-32.
- "Site and Stereo-selective Trans-Hydroboration of 1,3-Enynes Catalyzed by 1,4-Azaborine-Based Phosphine-Pd Complex." Xu, S.; Zhang, Y.; Li, B.; Liu, S.-Y. *Journal of the American Chemical Society*. 2016, 138, 14566-69.
- "Accessing 1,2-Substituted Cyclobutanes Through 1,2-Azaborine Photoisomerization." Giustra, Z.X.; Yang, X.; Chen, M.; Bettinger, H.F.; Liu, S.-Y. *Angewandte Chemie International Edition*. 2019, 58, 18918-22.
- "Synthesis and Characterization of an Unnatural Boron and Nitrogen-containing Tryptophan Analogue and its Incorporation into Proteins." Boknevitz, K.; Italia, J.S.; Li, B.; Chatterjee, A.; Liu, S.-Y. *Chemical Science*. 2019, 10, 4994-98.
- "The State of the Art in Azaborine Chemistry: New Synthetic Methods and Applications." Giustra, Z.X.; Liu, S.-Y. *Journal of the American Chemical Society*. 2018, 140, 1184-94.
- "The Least Stable Isomer of BN Naphthalene: Toward Predictive Trends for the Optoelectronic Properties of BN Acenes." Liu, Z.; Ishibashi, J.S.A.; Darrigan, C.; Dargelos, A.; Chrostowska, A.; Li, B.; Vasiliu, M.; Dixon, D.A.; Liu, S.-Y. *Journal of the American Chemical Society*. 2017, 139, 6082-85.
- "Medicinal Chemistry Profiling of Monocyclic 1,2-Azaborines." Zhao, P.; Nettleton, D.O.; Karki, R.; Zecri, F.J.; Liu, S.-Y. *ChemMedChem*. 2017, 12, 358-61.

UDAYAN MOHANTY

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RESEARCH INTERESTS

In the Mohanty lab, our aim is to tackle fundamentals in computational biophysics, materials chemistry, chemical biology, and theoretical physical chemistry. Problems of current interest are (1) large-scale conformational dynamics of the ribosome; (2) transport of divalent metal ions through MOF (metallic organic frameworks); (3) conformational dynamics of heparan sulfate (HS) mimetic oligomers; and (4) dynamics of supercooled liquids. In our research (highly collaborative with various scientists), we acquire scientific knowledge and insights that guide the development of new concepts and state-of-the-art computational and theoretical techniques.

SELECTED PUBLICATIONS

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- "A Metal-organic Framework Thin Film for Selective Mg2+ Transport." Luo, J.; Li, Y.; Zhang, H.; Wang, A.; Lo, W.S.; Dong, Q.; Wong, N.; Povinelli, C.; Shao, Y.; Chereddy, S.; Wunder, S.; Mohanty, U.; Tsung, C.K.; Wang, D. *Angewandte Chemie, International Edition*. 2019, 58, 15313-17.
- "Fluctuation Effects in the Adam-Gibbs Model of Cooperative Relaxation." Hutchison, C.; Bhattarai, A.; Wang, A.; Mohanty, U. *Journal of Physical Chemistry B*. 2019, 123, 8086-90.
- "RNA as a Complex Polymer with Coupled Dynamics of Ions and Water in the Outer Solvation Sphere." Lammert, H.; Wang, A.; Mohanty, U.; Onuchic, J. *Journal of Physical Chemistry B*. 2018, 122, 11218-27.
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RESEARCH INTERESTS

Synthetic organic chemistry has undergone a paradigm shift over the past 15 years with new metal-catalyzed transformations enabling bond formation in ways that chemists previously only dreamed about. Realizing the impact that new catalytic asymmetric reactions will have on the continued evolution of organic synthesis, we have focused our research on the development of new processes and on studying their utility in complex molecule synthesis. Our progress toward these goals depends upon expertise in many areas of chemistry including organometallic chemistry, physical organic chemistry, and synthetic organic chemistry.

Reactions of particular interest to our group are those that involve stereoselective transformations of simple unsaturated organic substrates. Along these lines, our group has recently developed enantioselective diboration, conjunctive cross coupling, and allyl-allyl coupling. These processes enable the simple, selective, and efficient construction of versatile chiral reaction products. To evaluate the utility of these processes we have engaged in the total synthesis of complex natural products. These stereochemically and functionally complex structures provide a challenging proving ground for new methods and have also inspired new directions in the development of catalytic transformations.

SELECTED PUBLICATIONS

- "Catalytic Conjunctive Cross-Coupling Enabled by Metal-Induced Metallate Rearrangement." Zhang, L.; Lovinger, G.J.; Edelstein, E.K.; Szymaniak, A.A.; Chierchia, M.P.; Morken, J.P. *Science*. 2016, 351, 70-74.
- "Hydroxyl-Directed Cross-Coupling: A Scalable Synthesis of Debromohamigeran E and Other Targets of Interest." Blaisdell, T.P.; Morken, J.P. *Journal of the American Chemical Society*. 2015, 137, 8712-15.
- "Asymmetric Synthesis From Terminal Alkenes by Diboration/Cross-Coupling Cascades." Mlynarski, S.N.; Schuster, C.S.; Morken, J.P. *Nature*. 2014, 505, 386-90.

FACULTY PROFILES

JIA NIU

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RESEARCH INTERESTS

Research in the Niu group consists of three distinct thrusts: (1) Bio-inspired precision macromolecules: A long-term goal of our research program is to develop precision synthetic macromolecules with chemically defined structures that mimic the structures and functions of biopolymers and are generated from biobased feedstocks. We expect these precision macromolecules to be used in a wide range of applications, including biomaterials, drug delivery and sustainable plastics. (2) Sulfation in biopolymers: plays a central role in many biological processes among proteins and carbohydrates, but their functional roles are not fully understood due to the highly heterogenicity of the sulfated biomolecules. A long-term goal of our group is to develop chemical tools for probing the functional roles of sulfation in biology. (3) Functional nucleic acids: Nucleic acids have emerged as a new class of functional materials in a wide range of diagnostic and therapeutic applications beyond carrying genetic information. As sequence-defined polymers, nucleic acids possess unique advantages such as ease of amplification, predictable thermal properties, programmable three-dimensional folding, and well-established technologies for intracellular trafficking. We are interested in developing next-generation nucleic acid polymers for advanced applications in biomedicine, such as immunomodulation and genome editing. Specifically, our research in this area is focused on two directions: the development of aptamer-integrated genome editing systems and functional xenobiotic nucleic acid aptamers for cell surface receptors. New technological platforms such as emulsion-based particle display selection and an CRISPR-mediated intracellular aptamer selection technology termed CRISPR-hybrid have been established to achieve these goals.

SELECTED PUBLICATIONS

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- "Precision Native Polysaccharides from Living Polymerization of Anhydrosugars." Wu, L.; Zhou, Z.; Sathe, D.; Zhou, J.; Reich, S.; Zhao, Z.; Wang, J.; Niu, J. *Nature Chemistry*. 2023. 15, 1276-84.
- "Fluorosulfate as a Latent Sulfate in Peptides and Proteins." Liu, C.; Liu, X.; Zhou, M.; Xia, C.; Lyu, Y.; Peng, Q.; Soni, C.; Zhou, Z.; Su, Q.; Wu, Y.; Weerapana, E.; Gao, J.; Chatterjee, A.; Lin, C.; Niu, J. *Journal of the American Chemical Society*. 2023, 145, 20189-95.
- "Degradable Vinyl Random Copolymers Via Photocontrolled Radical Ring-Opening Cascade Copolymerization." Wang, W.; Zhou, Z.; Sathe, D.; Tang, X.; Moran, S.; Jin, J.; Haeffner, F.; Wang, J.; Niu, J. *Angewandte Chemie International Edition*. 2022, 61, 8, e202113302.
- "'Click Handle'-Modified 2'-Deoxy-2'-Fluoroarabino Nucleic Acid as a Synthetic Genetic Polymer Capable of Post-Polymerization Functionalization." Wu. B.K.; Skrodzki, C.J.A.; Su, Q.; Lin, J.; Niu, J. *Chemical Science*. 2022, 13, 6873-81.
- "A General Approach to O-Sulfation via Sulfur(VI) Fluoride Exchange Reaction." Liu, C.; Yang, C.; Hwang, S.; Ferraro, L.S.; Flynn, P.J.; Niu, J. *Angewandte Chemie International Edition*. 2020, 59, 18435-41.
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- "Radical Cascade-Triggered Controlled Ring-Opening Polymerization Of Macrocyclic Monomers." Huang, H.; Sun, B.; Huang, Y.; Niu, J. *Journal of the American Chemical Society*. 2018, 140, 10402-06.

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RESEARCH INTERESTS

The interrelated aspects of our research program include introducing new chemical transformations, building complex molecules with these new reactions, and using these compounds to study cellular function.

The development of new reactions continues to be an important endeavor in organic chemistry. Our efforts have been directed toward discovering better ways of constructing medium-ring-containing compounds. Using novel transformations that build molecular complexity rapidly have allowed for the efficient construction of seven- and eight-membered ring, containing natural products. Moreover, we have also investigated whether there are new ways to discover new reactions. In this regard, we have found that rational selection protocols using combinatorial techniques can provide very attractive catalytic solutions to longstanding chemical problems.

Employing new reactions in the total synthesis of challenging molecules is not only important for organic chemistry; it also allows us to contribute to biological chemistry. Building molecules with unique or unusual biological activities can offer powerful new tools for studying biological systems. For example, we have used the synthesis of ilimaquinone, a marine sponge metabolite, to uncover previously unknown functional aspects of the Golgi apparatus. Similarly, other natural products currently under study will be used to provide a better understanding of the biological systems they influence. Combining organic chemistry with select techniques in protein chemistry and molecular and cellular biology yields a powerful multidisciplinary approach for advancing our understanding of various important scientific issues.

SELECTED PUBLICATIONS

- "Enantioselective Synthesis of Silyl Ethers through Catalytic Si-O Bond Formation." Hoveyda, A.H.; Snapper, M.L. In *Organosilicon Chemistry: Novel Approaches and Reactions*, eds. T. Hiyama and M. Oestreich. Wiley, 2019.
- "Nanothechnology: A Molecular Assembler." Kelly, T.R., Snapper, M.L. *Nature*. 2017, 549, 336.
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RESEARCH INTERESTS

Our research team engages in spectroscopic investigation of electro- and photo-catalytic interfaces that show potential for the synthesis of renewable fuels and high-value commodity chemicals. The development of renewable sources for these chemicals requires novel catalysts that efficiently and selectively enable the necessary chemical conversions. Our aim is to facilitate this development by identifying key descriptors of heterogeneous catalytic processes by carrying out case studies on prototypical catalytic systems. The exploration of the physical chemistry of electrocatalytic interfaces and the characterization of reaction intermiediates lies at the very core of this effort. To this end, we develop and apply vibrational techniques and couple them to complementary analytical methods to enable multimodal in situ probing of catalytic interfaces. Current research areas include electrochemical CO2 reduction, hydrogen evolution and photo- and electro-catalytic water oxidation.

SELECTED PUBLICATIONS

- "Correlating Hydration Free Energy and Specific Adsorption of Alkali Metal Cations During CO 2 Electroreduction on Au." Ovalle, V.J.; Hsu, Y.-S.; Agrawal, N.; Janik, M.J.; Waegle, M.M. *Nature Catalysis*. 2022, 5, 624-32.
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RESEARCH INTERESTS

The research in our lab bridges chemistry (in material synthesis), physics (property characterizations), and engineering (device constructions). We strive to meet the challenge of efficient solar energy conversion and utilization as well as advanced catalysis using novel materials. Equipped with state-of-the-art facilities, we design, synthesize, and study materials for catalysis applications. Our material design is guided by insights into the mechanisms of the various processes. The targeted applications include high-efficiency, low-cost solar fuel production, next generation batteries, and future commodity chemical production.

SELECTED PUBLICATIONS

- "Selective Methane Oxidation By Heterogenized Iridium Catalysts." Li, H.; Fei, M.; Troiano, J.L.; Ma, L.; Yan, X.; Tieu, P.; Yuan, Y.; Zhang, Y.; Liu, T.; Pan, X.; Brudvig, G.W.; Wang, D. *Journal of the American Chemical Society*. 2023, 145, 769-73.
- "Photocatalytic Depolymerization of Native Lignin Toward Chemically Recyclable Polymer Networks." Wang, H.; Giardino, G.J.; Chen, R.; Yang, C.; Niu, J.; Wang, D. *ACS Central Science*. 2023, 9, 48-55.
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FACULTY PROFILES

- "Role of H2O in CO2 Electrochemical Reduction as Studied in a Water-in-Salt System." Dong, Q.; Zhang, X.; He, D.; Lang, C.; Wang, D. *ACS Central Science*. 2019, 5, 1461.
- "Thin Film Photoelectrodes for Solar Water Splitting." He, Y.; Hamann, T.; Wang, D. *Chemical Society Review*. 2019, 48, 2182-215.
- "Selective CO Production by Photoelectrochemical Methane Oxidation on TiO2." Li, W.; He, D.; Hu, G.; Li, X.; Banerjee, G.; Li, J.; Lee, S.H.; Dong, Q.; Gao, T.; Brudvig, G.W.; Waegele, M.M.; Jiang, D.; Wang, D. *ACS Central Science*. 2018, 4, 631-37.
- "Stable Iridium Dinuclear Heterogeneous Catalysts Supported on Metal Oxide Substrate for Solar Water Oxidation." Zhao, Y.; Yang, K.; Wang, Z.; Yan, X.; Cao, S.; Ye, Y.; Dong, Q.; Zhang, X.; Thorne, J.E.; Jin, L.; Materna, K.; Trimpalis, A.; Bai, H.; Fakra, S.; Zhong, X.; Wang, P.; Pan, X.; Guo, J.; Flytzani-Stephanopoulos, M.; Brudvig, G.W.; Batista, V.S.; Wang, D. *Proceedings of the National Academy of Sciences of the USA*. 2018, 115, 2902-07.

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RESEARCH INTERESTS

Cysteine residues play key functional roles in protein activity, including nucleophilic and redox catalysis, metal-binding, and structural stabilization. Utilizing an interdisciplinary approach that merges synthetic chemistry, biochemistry, cell biology, and protein mass spectrometry, our group seeks to interrogate the role of cysteine-mediated protein activities in physiology and disease. We are particularly interested in generating selective chemical probes to monitor these activities and characterize specific cysteine-containing proteins as viable therapeutic targets. Furthermore, we are applying chemical proteomic technologies to identify and characterize novel functional cysteine residues in the human proteome. We focus on applying these chemical and mass-spectrometric tools to investigate dysregulated cysteine-mediated protein activities implicated in cancer, aging, and metabolic diseases and validate these proteins as potential therapeutic targets for these diseases.

SELECTED PUBLICATIONS

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- "Monitoring Iron-Sulfur Cluster Occupancy Across the E. Coli Proteome Using Chemoproteomic." Bak, D.W.; Weerapana, E. *Nature Chemical Biology*. 2023, 19, 356-66.
- "A Peptide-Crosslinking Approach Identifies HSPA8 and PFKL as Selective Interactors of an Actin-Derived Peptide Containing Reduced and Oxidized Methionine." Maurais, A; Weerapana, E. *RSC Chemical Biology*. 2022, 3, 1282-89.
- "Monitoring GAPDH Activity and Inhibition with Cysteine-reactive Chemical Probes." Canarelli, S.E.; Swalm. B.M.; Larson, E.T.; Morrison, M.J.; Weerapana, E. *RSC Chemical Biology*. 2022, 3, 972-82.
- "Generation of Recombinant Mammalian Selenoproteins through Genetic Code Expansion with Photocaged Selenocysteine." Peeler J.C.; Falco, J.A.; Kelemen, R.E.; Abo, M.; Edinger, L.C.; Chen, J.; Chatterjee, A.; Weerapana, E. *ACS Chemical Biology*. 2020, 19, 1535-40.
- "Profiling Cysteine Reactivity and Ooxidation in the Endoplasmic Reticulum." Bechtel, T.J.; Li, C.; Kisty. E.A.; Maurais, A.J.; Weerapana, E. *ACS Chemical Biology*. 2020, 15, 543-53.

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RESEARCH INTERESTS

Since Friedrich Wohler's groundbreaking synthesis of urea in 1828, organic synthesis over the past two centuries has predominantly relied on the exploration and utilization of chemical reactions rooted in two-electron heterolytic ionic chemistry. While one-electron homolytic radical chemistry is both rich in fundamental reactivities and attractive with practical advantages, the synthetic application of radical reactions has been long hampered by the formidable challenges associated with the control over reactivity and selectivity of high-energy radical intermediates. To fully harness the untapped potential of radical chemistry for organic synthesis, there is a pressing need to formulate radically different concepts and broadly applicable strategies to address these outstanding issues. In pursuit of this objective, we have been actively developing metalloradical catalysis (MRC) as a comprehensive framework to guide the design of general approaches for controlling over reactivity and stereoselectivity of homolytic radical reactions. Essentially, MRC exploits the potential of metal-centered radicals within open-shell metal complexes as one-electron catalysts for homolytic activation of substrates to generate metal-entangled organic radicals as the pivotal intermediates to govern

the reaction pathway and stereochemical course of subsequent catalytic radical processes. Different from the conventional two-electron catalysis by transition metal complexes, MRC operates through one-electron chemistry utilizing stepwise radical mechanisms. For achieving enantioselective radical reactions via MRC, we have designed D2 -symmetric chiral amidoporphyrins with tunable electronic, steric, and chiral environments as a general ligand flatform to support the development of metalloradical catalysts. These structurally well-defined chiral metalloradical catalysts, such as Co(II) and Fe(III) complexes, can effectively catalyze a wide range of important organic transformations through distinctive radical mechanisms that involve fundamentally new α-metalloalkyl, α-metalloaminyl, α-metalloxyl, and other metal-entangled organic radicals as the catalytic intermediates.

Guided by the principles and hypothesis of metalloradical catalysis, we have successfully developed a number of fundamentally new and practically attractive catalytic systems for stereoselective construction of synthetically useful organic molecules via homolytic radical chemistry. Examples include the asymmetric processes for radical olefin cyclopropanation, radical olefin aziridination, radical C–H alkylation, and radical C–H amination. Current ongoing research in the group is directed toward further exploration of new applications of metalloradical catalysis for solving other challenging organic transformations, including development of asymmetric catalytic systems for radical olefin epoxidation, radical C–H hydroxylation, and various types of radical cyclization reactions. We aim to utilize these catalytic radical reactions in a cascade manner for stereoselective synthesis of complex molecules and natural products.

SELECTED PUBLICATIONS

- "Metalloradical Catalysis: General Approach for Controlling Reactivity and Selectivity of Homolytic Radical Reactions." Lee, W.-C.C.; Zhang, X.P. *Angewandte Chemie International Edition*. 2024, 63, 20, e202320243.
- "New Mode of Asymmetric Induction for Enantioselective Radical N-Heterobicyclization Via Kinetically Stable Chiral Radical Center." Xu, H.; Wang, D.-S.; Zhu, Z.-Y.; Deb, A.; Zhang, X.P. *Chem*. 2024, 10, 283-98.
- "Iron(III) Porphyrin Complexes as Metalloradical Catalysts." Lee, W.-C. C.; Zhang, X.P. *Nature Chemistry*. 2023, 15, 1499-500.
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- "Metalloradical Approach for Concurrent Control in Intermolecular Radical Allylic C–H Amination." Xu, P.; Xie, J.-J.; Wang, D.-S.; Zhang, X.P. *Nature Chemistry*. 2023, 15, 498-507.
- "Asymmetric Radical Bicyclization for Stereoselective Construction of Tricyclic Chromanones and Chromanes with Fused Cyclopropanes." Lee, W.-C.C.; Wang, J.-Y.; Zhu, Y.-L.; Zhang, X.P. *Journal of the American Chemical Society*. 2023, 145, 11622-32.
- "Combined Radical and Ionic Approach for the Enantioselective Synthesis of β-Functionalized Amines from Alcohols." Lang, K.; Yang, H.; Lee, W.-C.C.; Zhang, X.P. *Nature Synthesis*. 2022, 1, 548-57.
- "Metalloradical Activation of In Situ-Generated a-Alkynyldiazomethanes for Asymmetric Radical Cyclopropanation of Alkenes." Ke, J.; Lee, W.-C.C.; Wang, X.-X.; Wang, Y.; Wen, X.; Zhang, X.P. *Journal of the American Chemical Society*. 2022, 144, 2368-78.
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RESEARCH INTERESTS

Nucleic acids are decorated with diverse types of chemical modifications that play essential regulatory functions in biology. Chemical modifications can change electrostatics, hydrophobicity, steric hindrance, and hydrogen bonding propensity of the modified moieties (i.e., nucleobase and sugar-phosphodiester backbone), altering nucleic acids structure, stability, and interactions with other molecules. Dysregulations of the chemical modification landscapes and their effector proteins have been found closely relevant in abnormal cellular functions, development disorders, and diseases. The Zhou research group focuses on developing and

FACULTY PROFILES

applying new technologies probe functional relevant RNA chemical modifications in the mammalian transcriptome at base resolution. We are interested in studying molecular mechanisms of biosynthesis and regulatory networks of RNA chemical modifications. We also develop platforms and tools to modulate transcript-specific RNA modification level in order to revert dysregulated epitranscriptome in diseases. We approach these interdisciplinary projects using directed evolution, protein engineering, RNA and enzyme biochemistry, mass spectrometry, next-generation sequencing, bioinformatics, and structural biology. Collectively, our research program aims to achieve in-depth understanding of regulatory mechanisms of epitranscriptome that can lead to discoveries of novel drug targets, and to diversify the tool box of gene therapy.

SELECTED PUBLICATIONS

- "Development of Mild Chemical Catalysis Conditions for M1a-to-M6a Rearrangement on RNA." Liu, H.; Zeng, T.; He, C.; Rawal, V.H.; Zhou, H.; Dickinson, B.C. *ACS Chemical Biology*. 2022, 17, 1334-42.
- "Evolution of A Reverse Transcriptase to Map N1-Methyladenosine in Human mRNA." Zhou, H.; Rauch, S.; Dai, Q.; Cui, X.; Zhang, Z.; Nachtergaele, S.; Sepich, C.; He, C.; Dickinson, B.C. *Nature Methods*. 2018, 16, 1281-88.
- "Resolving Crystallographic Ambiguity in Watson-Crick Versus Hoogsteen Base-pairing in a DNA-Protein Complex Using NMR and Site-specifically 13C/15N Labeled DNA." Zhou, H.; Sathyamoorthy, B.; Stelling, A.; Xu, Y.; Xue, Y.; Pigli, Y.Z.; Case, D.; Rice, P.A.; Al-Hashimi, H.M. *Biochemistry*. 2019, 58, 1963-74.
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- "New Insights into Hoogsteen Base Pairs in DNA Duplexes from a Structure-based Survey." Zhou, H.; Hintze B.J.; Kimsey, I.J.; Sathyamoorthy, B.; Yang S.; Richardson, J.S.; Al-Hashimi, H.M. *Nucleic Acids Research*. 2015, 43, 3420-33.

OUTCOMES

Recent Placements

The Department of Chemistry takes an active role in helping to place our students in attractive academic and non-academic positions. Our recent students' placements have included:

ACADEMIC PLACEMENTS

- Adelphi University
- Boston University
- Cornell University
- Brooklyn College
- Duke University
- Elon University
- Indiana University
- Kwangwoon University
- Loyola University, Chicago
- Massachusetts Institute of Technology
- Northeastern University
- Stanford University
- Texas A&M University
- Tufts University
- University of Basel
- University of California, Berkeley
- University of Maryland
- University of North Carolina, Chapel Hill
- University of Notre Dame
- University of St. Thomas
- Washington College
- Wellesley College

NON-ACADEMIC PLACEMENTS

- AbbVie
- Albany Molecular Research
- Alkermes
- Amgen
- Amprius, Inc.
- Applied Materials
- AstraZeneca Pharmaceuticals
- Biogen
- Bristol Myers Squibb
- Celgene
- Cytek Pharmaceuticals
- E-Ink Corporation
- Eli Lilly
- Enanta Pharmaceuticals
- Exelixis
- Hamilton Brook Smith Reynolds
- IBM
- Idenix Pharmaceuticals
- ImmunoGen
- Merck & Company
- Nano C, Inc.
- Novartis Institute of Biomedical Research
- Onyx Pharmaceuticals
- Pfizer Pharmaceuticals
- Syros Pharmaceuticals
- Vertex Pharmaceuticals

MORRISSEY COLLEGE OF ARTS AND SCIENCES

The oldest and largest of the University's eight schools and colleges, the Morrissey College of Arts and Sciences offers graduate programs in the humanities, social sciences, and natural sciences, leading to the degrees of Doctor of Philosophy, Master of Arts, and Master of Science. In addition, numerous dual-degree options are offered in cooperation with the Carroll School of Management, the Boston College Law School, the Lynch School of Education and Human Development, and the School of Social Work.

With approximately 900 graduate students and more than 500 full-time faculty, the Morrissey College of Arts and Sciences is small enough to know you as a person, but large enough to serve you and prepare you for a rewarding life and satisfying career.

Research Instrumentation and Facilities

The Department of Chemistry is housed in the 109,000-square-foot Eugene F. Merkert Chemistry Center, with modern classrooms, research laboratories, computation, instrumentation, and facilities all in a single building. Continual improvements ensure that our resources are kept up-to-date. The Merkert Center's sophisticated research facilities include a high-field Nuclear Magnetic Resonance (NMR) facility, featuring one 400 MHz, three 500 MHz, a 600 MHz NMR spectrometers, and an EMX-Plus EPR System; and an X-ray crystallography facility. Located nearby is a Mass Spectrometry facility that contains a wide range of state-of-the-art mass spectrometers and chromatographic system. Our facilities are run by full-time professional scientific staff.

All faculty members participate in the design of individual laboratories, built to accommodate state-of-the-art instrumentation and to provide flexibility for changing research needs. For example, an X-ray crystallography laboratory is fully equipped with a diffractometer and area detector, constant temperature rooms for crystal growth, and several VAX and silicon graphics computers for investigation of protein and small molecule structures. ESR spectroscopy, stopped-flow kinetics equipment, preparative centrifuges, scintillation counters, a DNA synthesizer, lasers, and ultra-high vacuum apparati are also available for use by individual research groups.

Other departmental instrumentation includes ReactIR, uV-Vis, atomic absorption, circular dichroism, GC- mass spectroscopy, gas and high performance liquid chromatography, magnetic susceptibility, electrochemistry, fermentation, and DNA- and protein-sequencing equipment. Faculty research collaborations with several area institutions afford our graduate students and postdoctoral staff easy access to additional state-of-the-art instrumentation.

Boston College is deeply committed to advancing research instrumentation and facilities in accordance with its strategic plan for strengthening the physical and life sciences. For example, a state-of-the-art clean room is available. Significant new research instrumentation is planned for the Department of Chemistry in the areas of chemical biology, X-ray, and advanced laser spectroscopy.

MORRISSEY COLLEGE OF ARTS AND SCIENCES

Academic Resources

GRADUATE RESEARCH SYMPOSIUM

Each October, the research activities of the Department of Chemistry are showcased during the Graduate Research Symposium. This event features seminar and poster presentations made by our graduate students. It is a highlight of the academic year, as it includes reports of the most exciting advances made in Department of Chemistry research groups during the preceding year.

GRADUATE STUDENT REPRESENTATIVES

Each year, several graduate students volunteer as department representatives and plan a variety of activities. In addition to planning the Graduate Research Symposium, they organize social activites such as movie nights and barbecues.

SEMINAR SERIES

The Department of Chemistry hosts a diverse seminar series that annually brings outstanding visiting scientists from around the world to campus for formal and informal interactions with all of the members of the department. Weekly seminars highlight nationally recognized speakers in organic, inorganic, physical, and biological chemistry. In addition, the seminar series is highlighted by our annual university lectureship, which invites acclaimed scientists to the department for a three-day visit that features stimulating daily seminars. Our recent university lecturers include Peter Schultz, Scripps Research Institute; Thomas Mallouk, University of Pennsylvania; Kyoko Nozaki, The University of Tokyo; John Bercaw, California Institute of Technology; Ben Feringa, University of Groningen; Dennis Dougherty, California Institute of Technology; and Robert Bergman, University of California, Berkeley.

Industrial Recruiting Program

The Industrial Recruiting Program annually brings companies to the Merkert Chemistry Center to interview eligible students for post-degree job opportunities. This program is available to all undergraduate and graduate students in the chemistry and biochemistry majors at Boston College. Graduate students who are in their final year of study may participate during their search for permanent positions as well as undergraduates who are seeking summer internships or research associate positions. When industrial laboratories visit the Department of Chemistry, their recruiter/scientist typically gives a presentation, conducts individual interviews with students, and meets with faculty.

A few of the corporate partners who recruit at BC include, but are not limited to: Amgen, Merck, Novartis, Takeda, Vertex, Biogen, Incyte, and Bristol Myers Squibb. For more information regarding this program, please contact the associate director for administration and graduate student services at 617-552-1735.

STUDENT LIFE AND CAMPUS RESOURCES

Boston College is located on the edge of one of the world's most vibrant cities. Just six miles from downtown Boston—an exciting and dynamic place to live and learn—Boston College is an easy car or "T" ride away from a booming center for trade, finance, research, and education.

Home to some of New England's most prestigious cultural landmarks, including the Museum of Fine Arts, the Isabella Stewart Gardner Museum, Boston Symphony Hall, and the Freedom Trail, Boston provides a rich environment for those passionate about art, music and history. For sports fans, Boston hosts a number of the country's greatest sports teams: the Celtics, Patriots, Bruins, and, of course, Fenway Park's beloved Red Sox. Found within a short drive from Boston are some of New England's best recreational sites, from the excellent skiing in New Hampshire to the pristine beaches of Cape Cod.

Boston also offers a wide range of family friendly attractions, including the Children's Museum, New England Aquarium, Franklin Park Zoo, and the Museum of Science. There are roughly 50 universities located in the Boston area, and the large student population adds to the city's intellectually rich and diverse community. Events, lectures, and reading groups hosted by world-renowned scholars abound on area campuses, providing abundant opportunities to meet and network with other graduate students and faculty throughout the Boston area.

The University

Boston College is a Jesuit university with 15,000 students, 880 full-time faculty, and more than 190,000 active alumni. Since its founding in 1863, the University has known extraordinary growth and change. From its beginnings as a small Jesuit college intended to provide higher education for Boston's largely immigrant Catholic population, Boston College has grown into a national institution of higher learning that is consistently ranked among the top universities in the nation. Boston College is ranked 36th among national universities by *U.S. News & World Report*.

Today, Boston College attracts scholars from all 50 states and over 80 countries, and confers more than 4,300 degrees annually in more than 50 fields through its eight schools and colleges. Its faculty members are committed to both teaching and research and have set new marks for research grants in each of the last 10 years. The University is committed to academic excellence. As part of its most recent strategic plan, Boston College is in the process of adding 100 new faculty positions, expanding faculty and graduate research, increasing student financial aid and widening opportunities in key undergraduate and graduate programs.

The University is comprised of the following colleges and schools: Morrissey College of Arts and Sciences, Carroll School of Management, Connell School of Nursing, Lynch School of Education and Human Development, Woods College of Advancing Studies, Boston College Law School, School of Social Work, and Clough School of Theology and Ministry.

STUDENT LIFE AND CAMPUS RESOURCES

General Resources

HOUSING

While on-campus housing is not available for graduate students, most choose to live in nearby apartments. The Office of Residential Life maintains an extensive database with available rental listings, roommates, and helpful local real estate agents. The best time to look for fall semester housing is June through the end of August. For spring semester housing, the best time to look is late November through the beginning of the second semester. Additionally, some graduate students may live on campus as resident assistants. Interested students should contact the Office of Residential Life.

JOHN COURTNEY MURRAY, S.J., GRADUATE STUDENT CENTER

One of only a handful of graduate student centers around the country, the Murray Graduate Student Center is dedicated to the support and enrichment of graduate student life at Boston College. Its primary purpose is to build a sense of community among the entire graduate student population and cultivate a sense of belonging to the University as a whole. Its amenities include study rooms, a computer lab, two smart televisions, kitchen, deck and patio space, complimentary coffee and tea, and more. Throughout the year, the center hosts programs organized by the Office of Graduate Student Life and graduate student groups. The Murray Graduate Student Center also maintains an active job board (available electronically), listing academic and non-academic opportunities for employment both on and off campus.

MCMULLEN MUSEUM OF ART

Serving as a dynamic educational resource for the national and international community, the McMullen Museum of Art showcases interdisciplinary exhibitions that ask innovative questions and break new ground in the display and scholarship of the works on view. The McMullen regularly offers exhibition-related programs, including musical and theatrical performances, films, gallery talks, symposia, lectures, readings, and receptions that draw students, faculty, alumni, and friends together for stimulating dialogue. Located on the Brighton campus, the McMullen Museum is free to all visitors.

CONNORS FAMILY LEARNING CENTER

Working closely with the Graduate School, the Connors Family Learning Center sponsors seminars, workshops, and discussions for graduate teaching assistants and teaching fellows on strategies for improving teaching effectiveness and student learning. Each fall, the Learning Center and the Graduate School hold a "Fall Teaching Orientation" workshop designed to help students prepare for teaching. The center also hosts ongoing seminars on college teaching, higher learning and academic life; assists graduate students in developing teaching portfolios; and provides class visits and teaching consultations, upon request. Through these and other activities, the Connors Family Learning Center plays an important role in enhancing the quality of academic life at Boston College.

MARGOT CONNELL RECREATION CENTER

The Margot Connell Recreation Center redefines the future of fitness and recreation at Boston College. The 244,000-square-foot, four-story structure offers our community an inspired space to play, pursue sports, gather with friends, and work out. This facility includes a fitness center, rock climbing wall, jogging track, aquatics center, wood-floor basketball courts, tennis courts, multi-activity courts, multi-purpose rooms for spin, yoga, and fitness classes, and so much more.

BOSTON COLLEGE CAREER CENTER

The Boston College Career Center works with graduate students at each step of their career development. Services include self-assessment, career counseling, various career development workshops, resume and cover letter critiques, and practice interviews. In addition to extensive workshop offerings, Career Center staff members are available throughout the year for one-on-one advising about any aspect of the career path. The Career Resource Library offers a wealth of resources, including books, periodicals, and online databases.

ADMISSION AND FINANCIAL INFORMATION

Student Profiles

Our graduate students come from across the United States and the globe. The program's demographics vary: currently it is 55 percent male, 45 percent female, and includes 45 percent international students. While some students enroll in the Ph.D. program immediately following their undergraduate studies, others begin their studies after working in a chemistry-related industry.

Admission Requirements

The application deadline for fall admission is December 15. Please visit bc.edu/mcgs for detailed information on how to apply.

Application requirements include:

Application Form:	Submitted online, via the MCGS website.
Application Fee:	$75, non-refundable.
Abstract of Courses Form:	A concise overview of background and related courses completed in an intended field or proposed area of study.
Official Transcripts:	Demonstrating coursework completed/degree conferral from all post-secondary institutions attended. Documents should show required courses: those normally required for a B.S. degree in chemistry, biochemistry, or chemical biology.
GRE General Test:	Official score report (optional).
GRE Subject Test:	Official score report (optional).
Three Letters of Recommendation:	From professors or supervisors.
Statement of Purpose:	A brief (one-two page) discussion of area(s) of research interest (organic, bioorganic, chemical biology, inorganic, theoretical, computational, physical, and biophysical). Additionally, identify specific research faculty who are of interest as future advisors.
Proof of English Proficiency: *(international only)*	Official TOEFL/IELTS score reports accepted.

Financial Assistance

DEPARTMENT FUNDING

First-year graduate students typically receive financial support as teaching assistants during the academic year, serving as instructors in undergraduate laboratories or as leaders of classroom discussion sections. For lab TAs, responsibilities include six to eight hours of weekly contact time in lab with students as well as grading lab reports. Discussion TAs attend class lectures, oversee four, one-hour discussion periods per week, and assist in grading quizzes and exams. All TAs hold office hours for their students. Teaching assistantships carry a nine-month stipend. Tuition-remission scholarships are also awarded to graduate students to cover the cost of program requirements.

Financial support during the summer is available to students as either research or teaching assistantships. Research assistantships are provided by individual professors from existing research grants, while teaching assistants are supported from departmental funds. Summer stipends cover three months' salary. The average yearly stipend for 2024–2025 is $40,000.

FEDERAL FINANCIAL AID

Graduate students can apply for federal financial aid using the FAFSA. The loans that may be available to graduate students are the Federal Direct Unsubsidized Stafford Loan and Perkins Loan, based on eligibility. If additional funds are needed, student may apply for a Grad Plus Loan. For more information, see the Graduate Financial Aid website at bc.edu/gradaid or contact the Graduate Financial Aid Office at 617-552-3300 or 800-294-0294.

OFFICE FOR SPONSORED PROGRAMS

The Office for Sponsored Programs (OSP) assists both faculty and graduate students in finding sources of external funding for their projects and provides advice in the development of proposals. OSP maintains a reference library of publications from both the public and private sectors listing funding sources for sponsored projects. In the recent past, graduate students have received research support from prominent agencies, corporations and organizations such as the Fulbright Commission, the Guggenheim Foundation, the National Science Foundation, the American Political Science Association, the American Chemical Society, and the American Association of University Women.

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