



GRADUATE STUDENT RESOURCE HANDBOOK

2024

WELCOME TO WASHU CHEMISTRY



*please contact Jasmyne Manuel-Nilsson
if any of the information is incorrect or
needs updating
jasmyn@wustl.edu*

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MESSAGE FROM THE DEPARTMENT CHAIR: DR. JEN HEEMSTRA



Welcome to WashU Chemistry!

We are thrilled that you have joined our department and are excited to partner with you in your PhD journey. No matter what your ultimate career goal is, our goal is to provide you with the environment, opportunities, and resources you need to grow as an independent scientist and pursue your career ambitions.

IMPORTANT THINGS TO KNOW

PARKING AND TRANSPORTATION

Parking & Transportation Office

Danforth University Center (DUC), room 239, Mon – Fri, 8:30 a.m. – 4 p.m.

Benefits-eligible WashU employees and full-time registered students are eligible for a [U-Pass](#), which allows individuals to ride the MetroLink and Metro buses for free. You can register for a U-Pass in-person or online
<https://parking.wustl.edu/items/metro-upass/>

If you wish to drive to campus, you can register for a parking pass. You can purchase a parking pass in-person or online <https://parking.wustl.edu/items/parking-permits/>
Please note: Parking passes cover specific parking Zones. The closest garage to the Chemistry buildings is the Millbrook Parking Garage which is in Zone 3. The Yellow Parking permit covers Zone 3.

LEARNING THE CHEMISTRY BUILDINGS

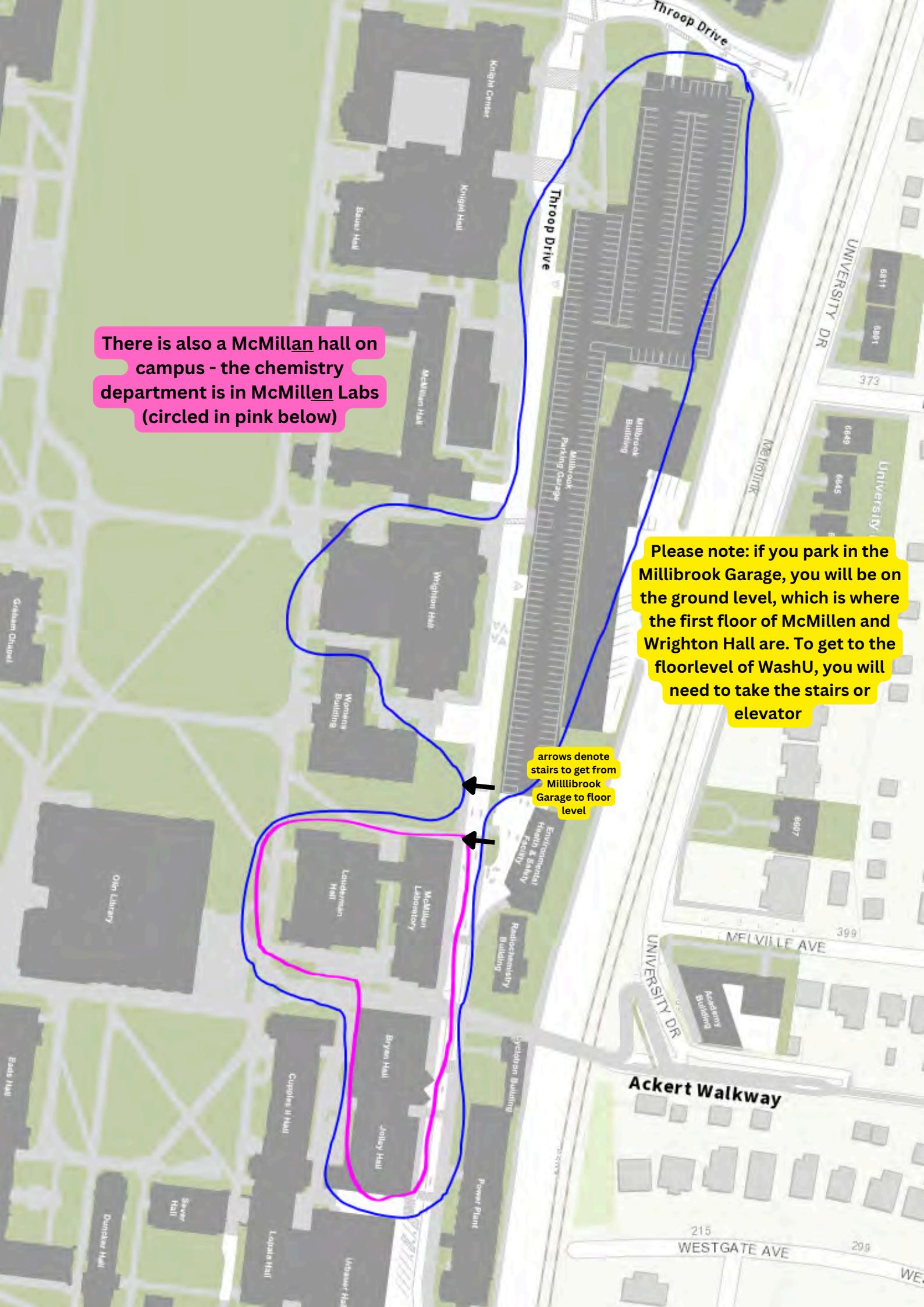
The main chemistry buildings are

- **Wrighton Hall**
 - The building contains research space, teaching laboratories, a 350-seat lecture hall, and other classrooms and lounges
 - If you are entering Wrighton Hall through the main entrance (floor level of WashU), you will technically be on the 3rd floor of Wrighton Hall
- **Chemistry Building Complex - Louderman Hall - McMillen Labs - Bryan Hall - Jolley Hall**
 - The Chemistry Building Complex includes Louderman Hall, McMillen Labs, Bryan Hall, and Jolley Hall, which are all connected through a series of hallways and staircases/elevators
 - **Please refer to the map when looking at the building complex to learn which hallways lead to which part of the building complex**
 - If you are entering the Chemistry building through the main entrance (floor level of WashU, facing towards Olin Library), you will be entering Louderman's 4th floor
 - Louderman is connected to McMillen Labs, McMillen Labs is connected to Bryan, and Bryan is connected to Jolley (you can ask Jasmyne for a brief tour of the spaces to see where everything connects)

There is also a McMillan hall on campus - the chemistry department is in McMillen Labs (circled in pink below)

Please note: if you park in the Millibrook Garage, you will be on the ground level, which is where the first floor of McMillen and Wrighton Hall are. To get to the floorlevel of WashU, you will need to take the stairs or elevator

arrows denote
stairs to get from
Millibrook
Garage to floor
level



CHEMISTRY ROOMS AND FACILITIES

IMPORTANT ROOMS TO KNOW

- **Storeroom:** Located on the 1st floor of McMillen Labs, you can take the stairs down or the elevator) please see the storeroom section below for more info
- **Tunnels:** There are tunnels that connect McMillen Labs to Wrighton Hall. The entrance to the tunnels is across from the storeroom. The tunnels are used for storage and easy transport access between the chemistry buildings. Please note that the tunnels are for Chemistry use only and you will need a specific key to access the tunnels. Ms. Jessie Owens will be able to assign you a key.
- **McMillen 311:** This is where guest speaker events and seminars occur. We have guest speakers and seminars every Thursday during the fall and spring semesters. Grad students also defend their thesis in this room.
- **Administrative Offices (located on the 5th floor of McMillen Labs):** This is where our Department Chair (Dr. Jen Heemstra) and a few staff members are located. If you are ever lost, confused, or not sure whom to connect with on a specific project, you can ask any of the staff members in these offices for help! They usually have snacks as well!!
- **Bryan Lounge:** Located on the 5th floor. The lounge is down the hallway where the Administrative Offices in McMillen Labs are. A lot of receptions and department events happen in the Bryan Lounge. There are tables available for students to relax and study. There are also additional tables and seating areas on the 4th floor of Bryan
- **Graduate Student Lounge:** Located in McMillen on the 4th floor. The space is equipped with seating areas, a refrigerator, and a microwave.
- **Rettner Gallery:** Located in Wrighton Hall on the 3rd floor. The Department occasionally hosts events in this space.
- **Wrighton 400:** Located in Wrighton Hall on the 4th floor. The Department occasionally hosts events in this space, but there are tables available for students to relax and study.

CHEMISTRY ROOMS AND FACILITIES

STOREROOM: MCMILLEN LABS RM 102

Open: Mon – Fri 8:00 a.m - 4:30 p.m., (closed from 12 p.m. - 1 p.m. for lunch)

Please make sure you stop by the storeroom and introduce yourself as a new grad student to Gerry Kohring, Michele Bigings, and Matt Beck (they're great!) and get a tour of the storeroom.

In the storeroom, you will find 1000+ different items that are ready for use. You can also get assistance with placing orders with outside vendors and the storeroom does all the shipping/receiving for the Department. New customers should complete the “new customer form” from below and bring it with them to the chemistry storeroom. At that time they will be entered as a customer authorized to shop on their labs account.

Please visit their website for more info: <https://chemistry.wustl.edu/chemistry-storeroom>

CHEMISTRY ROOMS AND FACILITIES

BIOMEDICAL MASS SPECTROMETRY FACILITY

- The Biomedical Mass Spectrometry (MS) research facility develops novel MS-based solutions to analytical challenges, and provides service, collaboration, and training for MS-based characterization, identification, and quantification of all biomolecular classes extracted from *in vitro* and *in vivo* model systems. The MS research facility supports integrated research programs in ion chemistry, protein biophysics, targeted and untargeted proteomics, focused on advancing MS platforms, software, and their analytical capabilities for expanding biological knowledge, and training the next generation of translational scientists interested in biomedical applications of MS.



- Basic Research** We are developing and applying methods in lipidomics, proteomics, protein biochemistry and biophysics, and biomarkers. We are also interested in new trap designs in FT-Ion Cyclotron Resonance and improved accurate mass measurements. We are developing new matrix and sample-handling strategies for MALDI and software for proteomics.

- Collaborative Research** We are excited to collaborate and utilize mass spectrometry for the identification, characterization, and quantitation of biomolecules including new and unusual lipids, the identification of proteins and their posttranslational modifications in proteomics, the analysis of mixtures of antigenic peptides in immunology, the determination of the composition of bacterial cell walls, and understanding the properties of proteins and their complexes with other molecules. Collaborations directed at the trace analysis of other biomolecules and in isotope ratio mass spectrometry is another goal.
- Service** We provide MALDI, ESI-MS accurate mass service, LC-MS, LC-MS/MS, denaturing and native ESI MS for large molecules (e.g., antibodies), DAR measurements, HDX MS, FPOP, chemical footprinting, and cross-linking MS. We also provide a variety of data analysis services using Protein Metrics software (e.g., proteomics database searching, intact analysis, drug-to-antibody ratio calculations). To arrange service projects, contact the facility staff. Training and
- Education** The resource provides training for users of mass spectrometry and education for graduate students and postdoctoral researchers. Prof. Michael Gross also teaches a graduate course in mass spectrometry (Chem 550) during alternate spring semesters.

CHEMISTRY ROOMS AND FACILITIES

NMR FACILITY

Staff

Dr. Manmilian Singh, Director

Dr. Jeff Kao, Senior NMR Spectroscopist

Instrumentation

- The Washington University High Resolution NMR Facility is located in Louderman 355 and Wrighton 240.
- The Facility currently houses six modern multi-nuclear spectrometers (field strengths from 300-600 MHz. The Facility's Agilent 600 MHz NMR is equipped with a cold probe which delivers unprecedented signal-to-noise or sensitivity gain over a room-temperature probe by drastically cutting down on background noise. The cold probe technology is used mostly for biomolecular NMR research, and it is also an excellent choice for certain challenging small molecule projects.
- The Varian Unity Inova 500 MHz NMR has been upgraded with a new Agilent DD2 console and thin shims. The state-of-the-art thin shims provide excellent control of field homogeneity, maintaining the same functionality, reliability, and purity of room temperature shims.

- 
- The Varian Mercury 300 MHz NMR located in Louderman 355 is available 24-7 for walk-up use, no reservations needed.
 - The Varian Inova 300 MHz NMR is located in Wrighton Hall, and is primarily dedicated for teaching efforts, but is also available for research samples. The magnet is equipped with an autosampler, which is used extensively in the data acquisition for the sophomore organic chemistry laboratory courses. The 300 MHz instrument is also used by advanced undergraduate and graduate courses: Chem 358 (Advanced Organic Chemistry Lab), Chem 445 (Instrumental Methods: Physical Chemistry Laboratory), Chem 470 (Inorganic Chemistry Laboratory), and Chem 558 (Spectral Methods in Organic Chemistry).
 - The Facility's newest instrument, a 400 MHz Bruker Biospin with autosampler, has recently been installed in Wrighton Hall. A Varian/Agilent Direct Drive 400 MHz instrument is located at the Medical School campus.

WHO TO CONTACT

CHEMISTRY STUDENT EMAILS

- Chris Thuet, (Computer Systems Manager), will add you to the grad student listserv. Please reach out to him if you do not receive department emails. Chris is also in charge of poster printing. Please introduce yourself to Chris and make sure that your email is working.
- cjthuet@wustl.edu | office: McMillen Labs 427
- **It is very important that you check your emails!!!!!!!**

WHO TO CONTACT

- **For all things about grad school, narrowing down your advisor, setting up your thesis, making sure you are on the right track with your program, etc.**
 - Barbara Taylor (Graduate Student Coordinator)
 - barbara22@wustl.edu | office: McMillen Labs 401
 - Dr. Tim Wencewicz (Director of Graduate Studies)
 - wencewicz@wustl.edu | Wrighton Hall 401c
- **IT issues and poster printing**
 - Chris Thuet (Computer Systems Manager) is in charge of all IT and poster-printing in the department.
 - cjthuet@wustl.edu | office: McMillen Labs 427
- **Assistance with Travel Funds**
 - The Chemistry Department and the Office of Graduate Studies will support each graduate student with \$400 to travel to a conference, meeting, etc. once per academic year if the student is going to present a talk or a poster at the meeting. Students should apply for the \$400 travel funds prior to traveling.
 - Barbara Taylor, Cindy Hodge, and V Watts are the individuals you should connect with.
 - Barbara Taylor (Graduate Student Coordinator)
 - barbara22@wustl.edu | office: McMillen Labs 401
 - Cindy Hodge (Manager of Finance & Administration)
 - hernkec@wustl.edu | office: McMillen Labs 519
 - V Watts (Accounting Assistant II)
 - vwatts@wustl.edu | office: McMillen 417
 - Please see the section on Travel for Graduate Students section for more info
- **Assistance with building maintenance/repairs**
 - Tay Birchfield (Chemistry Building Supervisor)
 - larvoyta@wustl.edu | McMillen Labs administrative offices 5th floor

WHO TO CONTACT

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- **Questions about Seminars or Guest Speakers**

- Julie Hamdi (Senior Lecturer)
 - Hamdi@wustl.edu | Louderman 450
- Jessie Owens (Front Office and Seminar Coordinator)
 - jessica@wustl.edu | McMillen Labs administrative offices 5th floor

- **Reserving a room and obtaining department keys**

- You will need to meet with Jessie Owens to get keys to different parts of the department including lab spaces, rooms, and the tunnels
- To check on room availability (to schedule a meeting, event, etc), you can utilize the Room Availability Calender on our website: <https://chemistry.wustl.edu/chemistry-room-calendar>
- To reserve the room, please contact Jessie Owens (Front Office and Seminar Coordinator)
 - jessica@wustl.edu | McMillen Labs administrative offices 5th floor

- **Social media, press releases/articles, Department website updates, DEI department events or trainings**

- Jasmyn Manuel-Nilsson (Community Engagement Coordinator)
 - jasmyn@wustl.edu | McMillen Labs 415
- Jasmyn can assist with social media, press releases, Department website updates, department events, or trainings. If you are interested in spearheading an Instagram or Twitter campaign, need a press release or article written for you or your lab group's accomplishment, need to update your profile on the website, or have ideas about different DEI events/trainings or things to enhance the culture of the chemistry department, please reach out.

- **If you are ever lost, confused, or unsure whom to connect with on a project or want a snack**

- Administrative Office Staff on McMillen Labs 5th floor!! You can ask any of the staff members in these offices for help! They know the ins and outs of the department and can point you in the correct direction.
- Kasey Driscoll (Assistant to the Chair and Administrative Coordinator)
 - kasey.driscoll@wustl.edu | McMillen Labs administrative offices 5th floor
- Jessie Owens (Front Office and Seminar Coordinator)
 - jessica@wustl.edu | McMillen Labs administrative offices 5th floor
- Brandon Hutchison (Coordinator of Undergraduate Studies)
 - b.hutchison@wustl.edu | McMillen Labs administrative offices 5th floor
- Tay Birchfield (Chemistry Building Supervisor)
 - larvoyta@wustl.edu | McMillen Labs administrative offices 5th floor

WHO TO CONTACT

GUIDE TO TRAVEL FOR GRADUATE STUDENTS

Before Traveling - Applying for Travel Funds

- The Chemistry Department and the Office of Graduate Studies will support each graduate student with \$400 to travel to a conference, meeting, etc., once per academic year if the student is going to present a talk or a poster at the meeting. Students should apply for the \$400 travel funds prior to traveling. Email either Barbara Taylor or Cindy Hodge with the following information to apply for the travel funds:
 - 1. Your student ID#
 - 2. Dates of travel
 - 3. Name of conference/meeting
 - 4. City/State/Country of the meeting
 - 5. Whether you are presenting a poster or giving a talk

Barbara or Cindy will submit the request for the travel funds once you've provided this information.

Before Traveling - International Travel

- The MyTrips International Travel Registry is a secure platform where faculty, staff, and student record travel itineraries and emergency contact information. MyTrips require travelers to create a one-time profile and then register the details of each trip. The registry allows WU to better assist you in emergencies of times of crisis while abroad. Register your trip with MyTrips before you travel (<https://global.wustl.edu/resources/travel-registry/>). If you fail to register your trip, WUSTL will not process your travel reimbursement for your international trip.

Considerations for Making Travel Arrangements

- 1. Air Travel
 - Federal regulations require travels to incur the lowest possible expense, and that air travel be on American-based airlines. FAQs about the FlyAmerica act:
https://financialservices.wustl.edu/wp-content/uploads/2016/11/SPA_WP_NP_TRAVEL_Fly-America-FAQ_rev3_9-2015.pdf
 - You should purchase the lowest economy fare available at the time of booking. Only economy class airfare will be reimbursed.
- Exceptions to purchasing the lowest available economy fare:
 - i. The lowest fare requires circuitous routing
 - ii. The lowest fare requires travel during unreasonable hours
 - iii. The lowest fare will excessively prolong travel
 - iv. The lowest fare would request in additional costs that would offset the transportation savings or
 - v. The lowest fare would offer accommodations not reasonably adequate for the traveler's medical needs

WHO TO CONTACT

GUIDE TO TRAVEL FOR GRADUATE STUDENTS

Considerations for Making Travel Arrangements (cont)

- You should prove that you're purchasing the lowest available economy fare by doing a print screen at the time of purchase
 - Upgrades are not allowed. Upgrades include (but are not limited to): upgrades in class, early-bird check-in, priority access seating, upgrades for preferred seats, etc. NOTE: Any fare other than "Wanna Get Away" on Southwest Airlines is considered an upgrade. If there are no "Wanna Get Away" fares available on Southwest Airlines when you're booking, be sure you document that by a print screen. Otherwise, you cannot be reimbursed for your air travel.
 - You must travel on an American-owned airline (e.g. American, Delta, United, Southwest, Frontier), even if a less costly non-American (e.g. British Airlines, Lufthansa, KLM) flight is available. Even if you're traveling internationally, you must use an American-owned airline.
 - **If you have any questions about purchasing your airfare, please ask Cindy Hodge or V Watts prior to making the purchase.**

Car Rentals

- To rent a car and have auto insurance coverage by WU car insurance, the car rental agreement must be purchased by PO.
- Contact Gerry Kohring for help with generating the PO for your car rental.
- Get a WU auto insurance card from either Cindy Hodge or V Watts before you leave for travel, and keep it with you while you're using the rental car. Return it to Cindy/V after your trip.
- Do not purchase additional auto insurance when renting a car. WU will not reimburse for it.

Personal Car Usage

- When a personal car is used, reimbursement is based on the current Internal Revenue Service (IRS) mileage rate
- You must maintain liability insurance on your car that meets the minimum statutory requirement for the state of your residency.
- If you choose to use a personal car for a work-related trip, then a more comprehensive review of all costs of flying versus driving needs to be considered. The reimbursement for the business use of a personal car is limited to the total costs associated with flying. You'll have to provide documentation to show that it is less expensive to use a personal car for a trip than to fly.
- You must print exact mileage from starting point to ending point from Google Maps and include this with your reimbursement request.

Personal Trip Add-Ons

- Please do not add personal trips before or after a business trip.

WHO TO CONTACT

GUIDE TO TRAVEL FOR GRADUATE STUDENTS

During Your Trip

- 1. Save ALL receipts, including receipts for cabs/Uber, dining expenses, parking expenses, etc.
 - Note: Uber has several classes of service. The only Uber services that can be reimbursed for are:
- UberX and UberPool. Unapproved Uber services are: Black Car, Taxi, SUV, and LUX
- 2. If meals are included in the costs of your conference/meeting, you cannot be reimbursed for any dining expenses. If you decide to visit a restaurant instead of eating the food provided by the conference, you cannot be reimbursed for that. You must include information from the conference (e.g. print screens from the conference website) that shows whether some/all/no meals are provided by the conference/meeting.
- 3. If you traveled internationally, you must document the exchange rate for the dates of travel using this website: www.oanda.com.
- 4. The exchange rate must be documented for each receipt. Print the exchange rate

After Your Trip - Filing for Reimbursement

- 1. Within 15 days of returning from your trip, you must file a travel expense statement with V Watts.
- 2. All trip expenses must be recorded on the travel expense statement, including pre-paid expenses.
- 3. Submit all original receipts (including airfare, lodging, meals, etc) with the travel expense statement.
- 4. Submit any print-screens that you took when you were booking your airline travel, to prove that you took the lowest rate economy fare available at time of purchase.
- 5. If you requested the \$400 in travel funds from the Chemistry Department, be sure to let V Watts know.
- 6. If you shared expenses with someone else from WU (e.g. you shared a rental car, a hotel room, a meal, etc.), you must let V Watts know. All travel reimbursement requests that are related due to shared expenses must be submitted before V Watts can process any of them for payment, because we are required to cross-reference them.
- 7. If your research advisor is paying a portion or all of your travel expenses, they will need to send an email to V Watts stating which fund(s) (GR#, PJ#, or GF#) to use for the reimbursement, and in what amount. Trip information - including conference name, dates, and location - should be included in this email.

GROUPS AND RESOURCES

CHEMISTRY GRAD STUDENT GROUPS

- There are multiple groups and committees grad students can join in order to get involved with the department. A few groups are listed below:
 - Safety Committee
 - Peer Mentoring
 - DEI Committee
 - Chemistry Graduate Student Advisory Committee (CGSAC)
 - Graduate Student Workshop Committee
 - Catalysts for Change (outreach)
 - Young Scientists Program (outreach)
 - BALSA (professional development)

CAMPUS WIDE GRAD STUDENT GROUPS AND RESOURCES

- Below is a list of graduate student groups and resources:
 - [Habif Health and Wellness](#): Habif is a full-service medical center with professional medical staff, same-day appointments for many issues, flu and other vaccination, nutrition services, contraception and reproductive health care, allergy injections, radiology facilities, an on-campus pharmacy and much more. In addition, Habif offers a suite of mental, sexual and emotional health resources.
 - [Gary M. Sumers Fitness Center](#): Located at the end of campus, this fitness center is the primary area for individual cardio and strength training. The west end of the Sumers Fitness Center is a cardio plaza with 65 cardio machines, including treadmills, ellipticals, stair steppers, lateral trainers, stationary bikes, and rowing machines. The east end of the Fitness Center houses the strength training area, which includes 41 strength stations and a full assortment of free weights. This area is also outfitted with a 12-foot medicine ball wall and a functional fitness rig. **Membership is free to full-time graduate students.**
 - [The Graduate Professional Council \(GPC\)](#) is the representative body to advocate for all 6,000+ graduate and professional students at WashU
 - [Graduate Student Groups](#): See universitywide graduate and professional student groups in WUGO: Washington University Student Group Organizer

GROUPS AND RESOURCES

CAMPUS WIDE GRAD STUDENT GROUPS AND RESOURCES

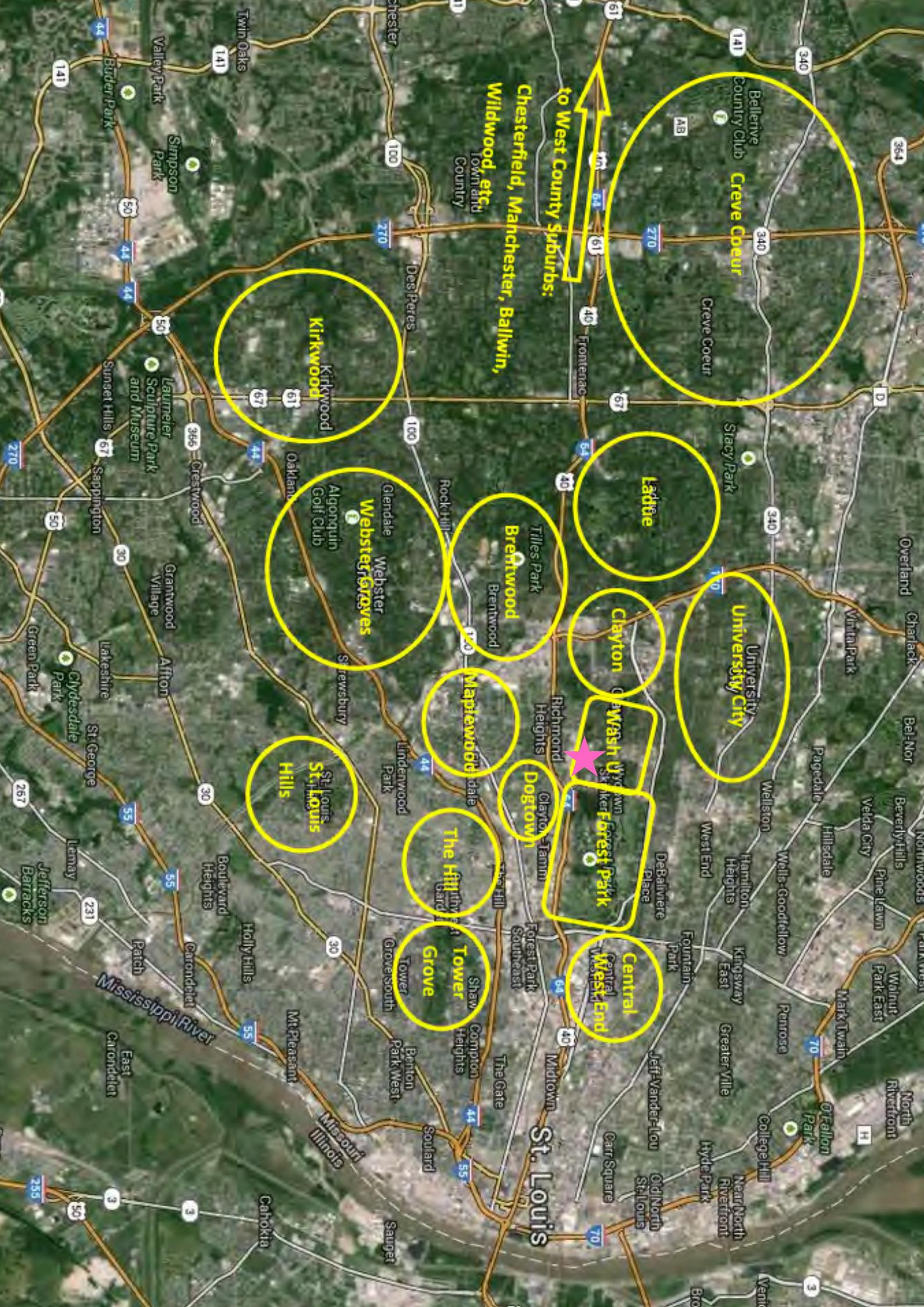
- **Below is a list of graduate student groups and resources:**
 - [The Graduate Center \(TGC\)](#): is a resource dedicated to graduate and professional students across all schools at Washington University. The Office of the Provost, university partners, and university-wide graduate student organizations host a variety of programming and workshops through the TGC. Topics include graduate student professional development, graduate student leadership, and interdisciplinary, academic, and personal development. The Graduate Center staff also advises university-wide graduate student organizations.
 - [Office of the Ombuds](#): The Offices of the Ombuds serve as confidential, independent and impartial resources that offer assistance in the informal resolution of university-related conflicts and advocate for fair treatment and process. Washington University has three separate ombuds offices dedicated to our faculty, staff, postdoctoral appointees, and medical and Graduate School students.
 - [Disability Resources](#): Disability Resources (DR) is the official resource for students on the Danforth Campus who have disabilities or suspected disabilities. DR is dedicated to ensuring that every student with a disability will have equal access to our campus and academic programs whether they are an undergraduate, graduate, professional, or continuing education student. We assist students individually by providing guidance and determining reasonable accommodations to remove barriers to access.
 - [Graduate Student and Postdoc Career Resources](#): The Career Center is here to support you in your career search, whether you are looking for an academic or non-academic job. We offer a range of services to assist you in your process:
 - [Office for International Students and Scholars](#): The OISS is here to support international students during their time at Washington University in St. Louis. Our services include immigration advising, orientation to the WashU and St. Louis communities, and other programs to help students thrive academically and socially and engage them in U.S. life and culture. This website has information and resources for international students enrolled in full-time in degree programs at WashU, international exchange students, and international alumni.
 - [Office of Military & Veteran Services](#): The Office of Military and Veteran Services is Washington University's focal point for military and veteran matters, to include transitioning military-connected students into higher education, providing and connecting students with programs and services, and partnering across campus and in the community.

FAMILY AND HOUSING INFO

FAMILY AND HOUSING - CAMPUS AND COMMUNITY RESOURCES

Housing Information

- The Quadrangle is off-campus housing dedicated to graduate students, staff, and faculty. You are able to filter your desired price range/beds/bathrooms/etc using their search function online:
<https://quadrangle.wustl.edu/properties/graduate/>
- WashU also partners with Parallel Properties (<https://www.rentparallel.com/>), Apartment Referral Services (<https://ars.wustl.edu/>), and Apartment List (<https://www.apartmentlist.com/mo/st-louis>)
- When filtering apartments by zip code, use zip codes 63130, 63110, and 63108 for listings near campus.
 - Please note: 63110 and 63108 are zip codes closest to WashU's Medical School Campus, which is only a 10-minute drive from the Danforth Campus.
 - The Medical Campus has a MetroLink station and is only one stop from the Danforth Campus. This is helpful if you do not have a car and will rely on the U-Pass.
- Additionally, there are many apartment complexes within the city's different neighborhoods. **Please take a look at the following map on the next page for a more detailed layout of STL neighborhoods.**
- Current grad students are a great resource to ask about housing. Feel free to connect with any of them (their emails are listed on the [Chemistry Department website](#)), or you can reach out to Jasmyne, and she will connect you with them.



FAMILY AND HOUSING INFO

FAMILY AND HOUSING - CAMPUS AND COMMUNITY RESOURCES

Family Care

- Lisa Eberle-Mayse, the Child and Family Care Facilitator in HR, is a great individual to connect with if you have any questions about family care, including childcare, early childhood education, schools, and adult/elder care. She connects faculty and staff with university resources and benefits, as well as other local resources, matching their individual family needs.
 - familycare@wustl.edu or lisae@wustl.edu
 - 314-935-3060
- **Child Daycare Subsidy**
 - Sponsored by Washington University in St. Louis, the purpose of the Child Daycare Subsidy is to help PhD student families meet the costs of child daycare while they pursue their studies. The amount of child daycare subsidy awarded to eligible applicants depends on their financial need, the number of children they have enrolled in child daycare facilities, their child daycare expenses, and available funding.
 - To learn more about eligibility, please visit: <https://provost.wustl.edu/child-daycare-subsidy/>
- **Day Care options**
 - Family Learning Center
 - Opened in September 2010, the Family Learning Center is a 19,900-square foot facility located on North Campus at 840 Rosedale Avenue in University City. The Center offers space for 156 children, ages six weeks to six years. Managed by Bright Horizons Family Solutions, the Family Learning Center serves the children of current University faculty, academic and non-academic staff for whom WashU is the primary employer, and the children of full-time graduate and professional students. Bright Horizons Family Solutions manages more than 700 child care and early education centers, including approximately 30 higher education clients.
 - <https://child-care-preschool.brighthorizons.com/MO/StLouis/wustl>

FAMILY AND HOUSING INFO

FAMILY AND HOUSING - CAMPUS AND COMMUNITY RESOURCES

Family Care

- Daycare options continued
 - University City Children's Center
 - Founded in 1970 by nine community synagogues and churches, today University City Children's Center (UCCC) reflects the founders' visionary desire to create a safe, nurturing environment where children from different socioeconomic, ethnic, and cultural backgrounds can learn and play together in an atmosphere that is respectful of diversity and individuality. UCCC is a 501 (c) (3) and opened with 28 children at Temple Shaare Emeth and was one of the very first programs to achieve accreditation with Missouri Voluntary Accreditation. UCCC now has the capacity to serve 164 children. We have a growing reputation as a thought-leader in early childhood education and human development. Our notions of innovation and creative thinking in the classroom drive the continuous improvement of our program, evolving into the LUME Approach. We are able to serve a large group of underserved children within a highly diverse environment because of our ability to provide financial assistance to our families, and are successful because of our ability to put sound child development theory into practice.
 - <https://www.uccc.org/>
 - phone: (314) 726-0148

FAMILY AND HOUSING INFO

FAMILY AND HOUSING - CAMPUS AND COMMUNITY RESOURCES

On campus lactation rooms

- To locate a lactation room, please review the list provided below. For questions or to schedule room usage where required, please contact the specified individual(s).

Building	Room Location	Facilities	Access Information and Contact
Brauer Hall (Danforth Campus)	Third floor (west), Room 3013A	Private room with toilet, mirror, sink, and electrical outlets	For access, contact Dean of Engineering office at 314-935-6350 or via email: eng-dean-admin@wustl.edu .
Busch Hall (Danforth Campus)	Lower level, corridor connecting to Brookings Hall	Small room with privacy lock, chair, diaper changing station, mirror, sink, and electrical outlets	Open and available for unscheduled use
Cupples II (Danforth Campus)	Third Floor East	Room with electrical outlets, sink, toilet, and chair	Open and available for unscheduled use
Danforth University Center (Danforth Campus)	Third floor next to south elevator, Room 304	Small room with privacy lock, sink, chair, mirror, and electrical outlets	Locked, but available for unscheduled use during building hours as posted online . For key access, please visit the student employee at the Fun Room information desk on the second floor or DUC 160.
Gregg Residence Hall (South 40, Danforth Campus)	Ground floor, Cornerstone, Room 00125	Small room with privacy lock, chair, and electrical outlets	Contact information pending
Family Learning Center (North Campus)		Private lactation room	Reserved for parents of children enrolled at the Family Learning Center

FAMILY AND HOUSING INFO

FAMILY AND HOUSING - CAMPUS AND COMMUNITY RESOURCES

On campus lactation rooms

- To locate a lactation room, please review the list provided below. For questions or to schedule room usage where required, please contact the specified individual(s).

Building	Room Location	Facilities	Access Information and Contact
Knight Center	First floor, Room 169	Private room with a privacy lock	Contact Shante Redden at 935-9253 or Olin Business School General Services at 314-935- 7788 to schedule.
Simon Hall	Second floor, Room 282	Private room with a privacy lock	Contact Shante Redden at 935-9253 or Olin Business School General Services at 935-7788 to schedule.
Umrath Hall (Danforth Campus)	Room 020	Room with electrical outlets, changing table, sink, and chair	Open and available for unscheduled use
West Campus	Lower level, east building, Room 42A (view map)	Small room with privacy lock, chair, table, and electrical outlets	Open and available for unscheduled use for active employees with a WashU ID card. Swipe card for access.
Women's Building (Danforth Campus)	Lower Level (east), near restrooms across from Campus Card Services	Private room with a chair, sink and electrical outlets	Open and available for unscheduled use.

LIVING IN STL

GETTING A MISSOURI DRIVER LICENSE

- A new Missouri resident with an out-of-state driver license or nondriver ID, either valid or expired no more than 184 days, must provide acceptable documents of the following:
 - Proof of Identity;
 - Date of Lawful Status;
 - Proof of Social Security number; and
 - Proof of Missouri residential address.
- NOTE: A new applicant requesting a REAL ID-compliant document, a Commercial Driver License or a Commercial Learner's Permit must submit two acceptable documents as proof of Missouri residency and state of domicile.
 - **Source:** <https://dor.mo.gov/driver-license/issuance/required-documents-checklist.html#resident>

REGISTERING YOUR CAR

- This is kind of a painful process!!! Please visit <https://dor.mo.gov/motor-vehicle/titling-registration/> for more info as there are many nuances/exceptions
- You have 30 days from the date of becoming a Missouri resident to title your vehicle.
 - To obtain a Missouri title and registration (license plates) on a motor vehicle currently titled in another state, you must submit the following:
 - Original title, or proof of ownership in accordance with the laws of your previous state where the vehicle is currently titled in your name;
 - A signed **Application for Missouri Title and License (Form 108) PDF Document**;
 - **Identification number and odometer (ID/OD) inspection.** All motor vehicles previously titled in another state must be inspected to verify the vehicle identification number and odometer reading of the vehicle. This inspection can be completed by a Missouri authorized inspection station. A Missouri **safety inspection** will satisfy this requirement;
 - Additional documentation may be requested at the time of titling;
 - **A current insurance identification card** (original, copy, or electronic if legible) or other proof of **financial responsibility**;
 - **Statement of non-assessment** from your Missouri county of residence (or City of St. Louis) assessor's office showing you do not owe personal property taxes in the county (or City of St. Louis).
 - *A Missouri **safety inspection** not more than 60 days old;
 - *An **emissions inspection** not more than 60 days old, if you reside in St. Louis City or the following counties: Jefferson, St. Charles, or St. Louis, if applicable.
- **Source:** <https://dor.mo.gov/driver-license/issuance/required-documents-checklist.html#resident>

LIVING IN STL



REGISTERING TO VOTE

- Start your online registration on [Missouri's election website](#).
 - You can also register to vote by mail or in person on [Missouri's election website](#).
 - Voter registration deadlines
 - **Online registration deadline:** 27 days before Election Day
 - **Register by mail deadline:** Must be postmarked 27 days before Election Day
 - **In person registration deadline:** 27 days before Election Day
 - **Source:** <https://vote.gov/register/mo/>

REGISTER YOUR PET WITH THE CITY

- Every person who owns, keeps, or harbors any dog, puppy, cat, or kitten in or around their home, place of business, or other premises within the City is responsible for having that animal vaccinated against rabies and registered with the City. No dog or cat shall be permitted to remain within city limits without the required vaccination and registration. Failure to maintain the required vaccination and registration can result in a ticket and a fine.
 - **For more information, please visit** <https://www.stlouis-mo.gov/government/departments/health/animal-care-control/pet-registration.cfm>

FACULTY RESEARCH BIOS

PLEASE NOTE: not all faculty members are accepting graduate students at this time, and their current projects may be different - please contact them beforehand or check their page on the Department Website for the most updated info



The Department of Chemistry offers a PhD in Chemistry that prepares scientists for careers in research and teaching. The program offers pathways for graduate studies that span biological, organic, inorganic, physical, and nuclear chemistry. Key to the success of the students and the Chemistry PhD program is the strong interpersonal connections that develop between our students and the faculty and that often lead to new research directions and bridges being built between disciplines. As a result, doctoral students commonly pursue research at the interface of two or more subfields of chemistry.

During the first semester of residence in the program, students are given the opportunity to explore research options within the department and to identify research mentors with common interests. The PhD requirements are kept to a minimum so that students can focus on scientific discovery and building skillsets for successful careers.

Students are taught by research-active faculty in the classroom and in the laboratory so that modern concepts with applications in scientific discovery prepare students for careers in science. Most of the research groups in Chemistry are small enough so that faculty are intimately involved with ongoing research and progress of the students.



ASSOCIATE PROFESSOR

Organic, Polymer, and Materials Chemistry

Jonathan C. Barnes

HHMI Postdoctoral Fellow, MIT (2014-2016); PhD DoD NDSEG Fellow, Northwestern University (2014); BS/MS University of Kentucky (2006).

ACS PMSE Young Investigator (2020); Polymer Chemistry, Emerging Investigator (2020); Supramolecular Chemistry, Emerging Supramolecular Chemist in the US (2019); Kavli Fellow - Kavli Foundation / US National Academy of Sciences (2019); Young Investigator Award (Cancer Research Foundation); Packard Fellowship for Science and Engineering (2017); Foresight Fellow - Synthetic Polymer Chemistry (2017); IUPAC-SOLVAY International Award for Young Chemists (2015); 2013 Foresight Institute Distinguished Student Award (2014); DoE Innovations in Fuel Cycle Research Award (2013); Northwestern

The overarching goal of the Barnes group is to develop next-generation polymeric materials that can be programmed at the (macro)molecular level with precise functions, resulting in advanced materials that have enhanced properties for a broad range of applications. We design and synthesize functional monomers, polymers, and crosslinkers with non-covalent bonding capabilities – i.e., supramolecular properties – that adopt unique pathways of self-assembly and/or activation. Ultimately, the Barnes group seeks to find solutions to problems at the interface of chemistry, engineering, materials science, biology, and medicine.

The Barnes research group employs a multi-disciplinary approach towards research challenges in the areas of stimuli-responsive polymers and hydrogels, nanoparticle-based combination drug delivery, biomaterials, and topologically complex polymers and materials. The “keystone” of our research program is synthetic organic chemistry, which is central to the preparation of all functional materials in our group. Supramolecular and polymer chemistries are directly associated with this keystone, and together, all three areas represent the foundation of the research group. We aim to build on this foundation by constructing novel ‘smart’ materials with well-defined functions – for both fundamental and applied purposes – that will ultimately lead us down research pathways in the areas of nanomaterials, biomedical engineering, and inorganic and environmental chemistries.

Selected Publications

- Amir, F.; Gruschka, M.; Colley, N. D.; Li, L.; Linder, H. R.; Sell, S. A.; **Barnes, J. C.*** Dynamic, Multimodal Hydrogel Actuators Using Porphyrin-Based Visible Light Photoredox Catalysis in a Thermoresponsive Polymer Network. *Chem. Sci.* **2020**, *11*, 10910–10920. *Outside Front Cover*.
- Colley, N. D.; Nosiglia, M. A.; Li, L.; Amir, F.; Chang, C.; Fisher, J. A.; **Barnes, J. C.*** One-Pot Synthesis of a Linear [4]Catenate Using Orthogonal Metal Templatation and Ring-Closing Metathesis. *Inorg. Chem.* **2020**, *59*, 10450–10460.
- Delawder, A. O.; **Barnes, J. C.*** Precise patterning driven by droplets. *Nature Chem., News & Views* **2020**, *12*, 328–330.
- Li, R.; Li, X.; Zhang, Y.; Delawder, A. O.; Colley, N. D.; Whiting, E.; **Barnes, J. C.*** Diblock Brush-Arm Star Copolymers via a Core-First/Graft-From Approach Using γ -Cyclodextrin and ROMP: A Modular Platform for Drug Delivery. *Polym. Chem.* **2020**, DOI: 10.1039/C9PY01146C. Part of the ‘Polymer Chemistry Emerging Investigators 2020’ issue.
- Delawder, A. O.; Natraj, A.; Colley, N. D.; Saak, T.; Greene, A. F.; **Barnes, J. C.*** Synthesis, Self-Assembly, and Photomechanical Actuator Performance of a Sequence-Defined Polyviologen Macrocrosslinker. *Supramol. Chem.* **2019**, *31*, 523–531. Part of the ‘Emerging Supramolecular Chemists in the United States’ special issue.
- Amir, F.; Liles, K. P.; Delawder, A. O.; Colley, N. D.; Palmquist, M. S.; Linder, H. R.; Sell, S. A.; **Barnes, J. C.*** Reversible Hydrogel Photopatterning: Spatial and Temporal Control Over Gel Mechanical Properties Using Visible-Light Photoredox Catalysis. *ACS Appl. Mater. Interfaces* **2019**, *11*, 24627–24638.
- Liles, K. P.; Greene, A. F.; Danielson, M. K.; Colley, N. D.; Wollen, A.; Fisher, J. A.; **Barnes, J. C.*** Photoredox-based Actuation of an Artificial Molecular Muscle. *Macromol. Rapid Commun.* **2018**, 1700781.
- Greene, A. F.; Danielson, M.; Liles, K. P.; Delawder, A. O.; Li, X.; Natraj, A.; Wollen, A.; **Barnes, J. C.*** Redox-Responsive Artificial Molecular Muscles: Reversible Radical-Based Self-Assembly for Actuating Hydrogels. *Chem. Mater.* **2017**, *29*, 9498–9508.
- **Barnes, J. C.**; Bruno, P.; Nguyen, H. V.-T.; Liao, L.; Liu, J.; Hemann, M. T.; Johnson, J. A. Using an RNAi Signature Assay to Guide the Design of Three-Drug Conjugated Nanoparticles with Validated Mechanisms, *In Vivo* Efficacy, and Low Toxicity. *J. Am. Chem. Soc.* **2016**, *138*, 12494–12501.
- **Barnes, J. C.**; Ehrlich, D. J.; Gao, A. X.; Leibfarth, F. A.; Jiang, Y.; Zhou, E.; Jamison, T. F.; Johnson, J. A. Iterative Exponential Growth of Stereo- and Sequence-Controlled Polymers. *Nature Chem.* **2015**, *7*, 810–815. **Highlighted in RSC’s Chemistry World, Nature.**
- **Barnes, J. C.**; Dale, E. J.; Prokofjevs, A.; Narayanan, A.; Gibbs-Hall, I. C.; Jurićek, M.; Stern, C. L.; Sarjeant, A. A.; Botros, Y. Y.; Stupp, S. I.; Stoddart, J. F. Semiconducting Single Crystals Comprising Segregated Arrays of Complexes of C₆₀. *J. Am. Chem. Soc.* **2015**, *137*, 2392–2399.

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ASSOCIATE PROFESSOR

Organic Chemistry

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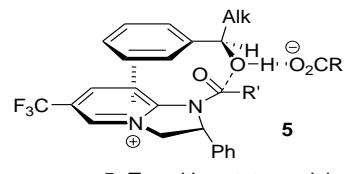
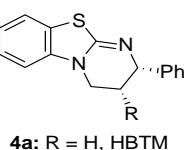
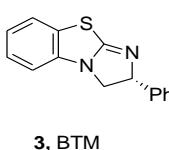
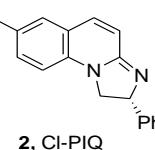
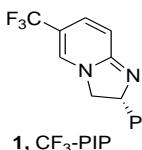
Vladimir Birman

Postdoctoral Fellow, Columbia University (2000-3); Ph.D., The University of Chicago (2000); B.S., University of North Carolina at Charlotte (1995).

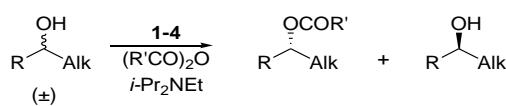
Our efforts currently focus on the rational design of new enantioselective organocatalysts, development of their applications in asymmetric synthesis, and elucidation of the origin of enantioselectivity in catalytic processes. Our group has developed Amidine-Based Catalysts **1-4** (ABCs) illustrated below. These easily synthesized catalysts display remarkable versatility and enantioselectivity in a variety of asymmetric acyl substitution reactions. For example, they are highly effective in promoting kinetic resolution (KR) of several classes of alcohols. In addition, we have discovered that lactams and thiolactams can be resolved in an analogous fashion via enantioselective N-acylation. The asymmetric induction observed in all these cases is explained in terms of π -interactions, as illustrated by transition state model **5**. ABCs also catalyze enantioselective alcoholysis of chiral acyl donors, e.g., KR of N-aryl- β -lactams and Dynamic Kinetic Resolution (DKR) of azlactones. We have also discovered that the DKR of azlactones is effectively promoted by a different class of catalysts, chiral Brønsted acids. To learn about additional directions of our research, please visit our web page: <http://www.chemistry.wustl.edu/people/vladimir-birman>

Scheme 1: ABCs and their applications

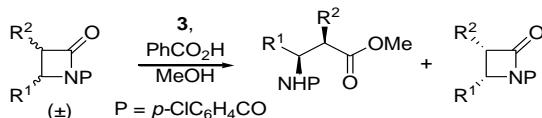
Amidine-Based Catalysts



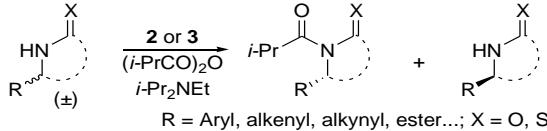
Enantioselective O-acylation



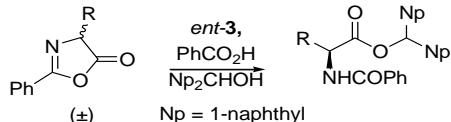
KR of N-aryl- β -lactams



Enantioselective N-acylation



DKR of azlactones



Selected Publications

- Yin, J.; Birman, V. B. Org. Lett. 2022, 24, 8759-8763. DOI: 10.1021/acs.orglett.2c03450 (b) Yin, J.; Birman, V. B. J. Org. Chem. 2022, 87, 15744-15753. DOI: 10.1021/acs.joc.2c01445
- J. Yin, A.N. Khalilov, P. Muthupandi, R. Ladd, and V.B. Birman*, "Phenazine-1,6-dicarboxamides: Redox-Responsive Molecular Switches", *J. Am. Chem. Soc.*, **142**, 60-3 (2020).
- M.R. Straub and V.B. Birman*, "Organocatalytic Enantioselective Synthesis of α -Fluoro- β -amino Acid Derivatives", *Organic Letters*, **20**, 7550-3 (2018).
- N.A. Ahlemeyer, E.V. Streff, P. Muthupandi, and V.B. Birman*, "Dramatic Acceleration of an Acyl Transfer-Initiated Cascade by Using Electron-Rich Amidine-Based Catalysts", *Organic Letters*, **19**, 6486-9 (2017).
- N.A. Ahlemeyer and V.B. Birman*, "Asymmetric Catalytic Synthesis of Thiochromenes via an Acyl Transfer-Initiated Cascade", *Organic Letters*, **18**, 3454-7 (2016).
- V.B. Birman* and X. Li, "Benzotetramisole: A Remarkably Enantioselective Acyl Transfer Catalyst", *Organic Letters*, **8**, 1351-4 (2006).
- X. Li, H. Jiang, E.W. Uffman, L. Guo, Y. Zhang, X. Yang, V.B. Birman*, "Kinetic Resolution of Secondary Alcohols Using Amidine Based Catalysts", *J. Org. Chem.*, **77**, 1722 (2012).
- X. Yang, V.D. Bumbu, P. Liu, X. Li, H. Jiang, E.W. Uffman, L. Guo, W. Zhang, X. Jiang, K.N. Houk*, and V.B. Birman*, "Catalytic, Enantioselective N-Acylation of Lactams and Thiolactams Using Amidine-Based Catalysts", *J. Am. Chem. Soc.*, **134**, 17605-12 (2012).
- X. Li, P. Liu, K.N. Houk*, V.B. Birman*, "Origin of Enantioselectivity in CF₃-PIP-Catalyzed Kinetic Resolution of Secondary Benzylic Alcohols", *J. Am. Chem. Soc.*, **130**, 13836 (2008).



PROFESSOR

Organometallic/Inorganic Chemistry

John R. Bleeeke



Postdoctoral Fellow, University of California-Berkeley and Lawrence Berkeley Lab (1981); Ph.D., Cornell University (1981); B.A., summa cum laude, Carthage College (1976).

Panelist, NSF Graduate Fellowship Selection Committee (2008—present); Member, Executive Committee, Pew Midstates Consortium for Math and Science (1989-present); Director, Washington University Beckman Scholars Program (2006-9); Editorial Advisory Board, *Organometallics* (1993-5); NSF Predoctoral Fellow (1976-9).

Since joining the chemistry faculty in 1981, Profesor Bleeeke has established a nationally and internationally recognized research program in the area of transition metal organometallic chemistry. He is particularly well known for his research with metallabenzenes and other aromatic metallacycles.

Ever since Kekule's intuitive idea on the structure of benzene, "aromaticity" has been one of the most fascinating and provocative research topics in chemistry. While benzene is the archetypical aromatic compound, it is now well known that heterocyclic analogues of benzene containing N, O, P or S also exhibit aromatic properties. In contrast very little is known about metallacyclic benzenoid compounds, i.e., benzene analogues in which a CH group has been formally replaced by a transition metal and its associated ligands. Such "metallabenzenes" represent a fundamentally new class of aromatic compounds in which metal d orbitals participate fully with carbon p orbitals in the formation of ring pi-bonds. We have succeeded in synthesizing metallabenzenes using an approach that employs pentadienyl reagents as the source of ring carbon atoms and C-H bond activation in the key ring-forming step. Using this strategy, we have synthesized red crystalline "iridabenzene" (see figure 1) in high yield.

X-ray crystallography of I has confirmed the presence of a fully delocalized (and almost planar) metallacyclic ring, while the ¹H NMR spectrum exhibits downfield chemical shifts, consistent with the presence of an aromatic ring current. Iridabenzene I exhibits a rich and varied reaction chemistry. Some of these reactions are typical of conventional organic arenes while others differ sharply due to the powerful influence of the transition metal center.

More recently, we have begun to study the synthesis of heteroatom-containing analogues of I, species such as iridafuran, iridapyrylium, iridathiophene, iridathienobenzene, and iridapyrrole. Our goal is to generate a family of closely-related molecules, enabling us to assess the effects of ring size and heteroatom incorporation on stability, structure, spectroscopy, and reactivity.

Selected Publications

- J.R. Bleeeke, W. Anutrasakda, and N.P. Rath, "Synthesis, Structure, Spectroscopy, and Reactivity of Azapentadienyl-Cobalt-Phosphine Complexes," *Organometallics*, **31**, 2219-2230 (2012).
- J.R. Bleeeke, P. Putprasert, T. Thanathanthanachon, and N.P. Rath, "Synthesis and Characterization of Fused-Ring Iridapyrroles," *Organometallics*, **27**, 5744-5747 (2008).
- J.R. Bleeeke, "Aromatic Iridacycles," *Acc. Chem. Res.*, **40**, 1035-1047 (2007).
- J.R. Bleeeke, "Synthesis and Reactivity of Heteropentadienyl-Transition-Metal Complexes," *Organometallics*, **24**, 5190-5207 (2005).

ASSISTANT PROFESSOR

Physical Chemistry

Joseph A. Fournier

Postdoctoral Fellow, Department of Chemistry at the University of Chicago (2015-2018); Ph.D., Yale University (2015); B.S., University of Connecticut (2010).

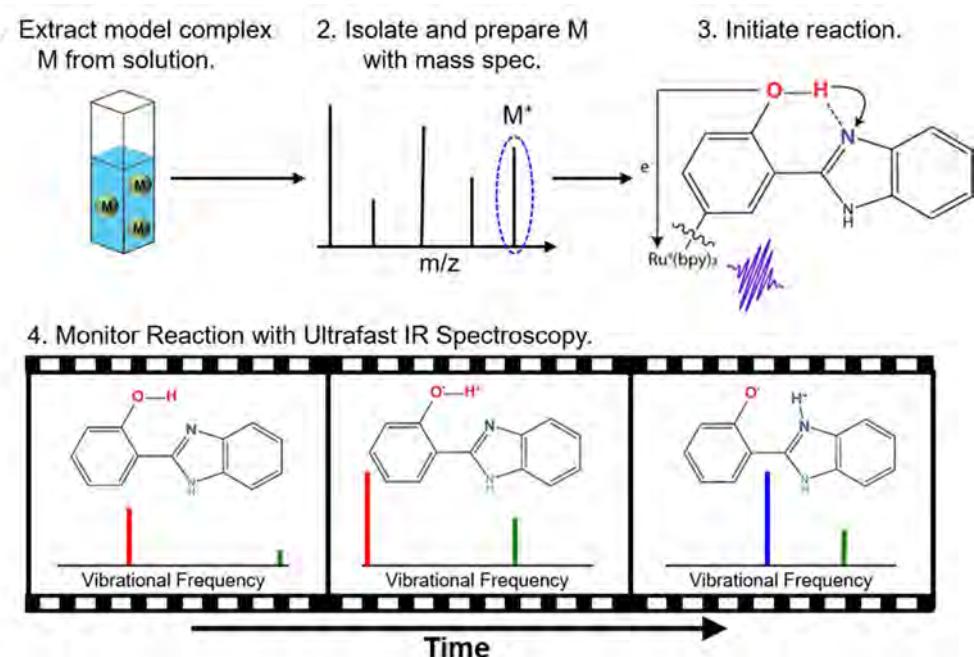
NSF Career Award (2021); Arnold O. Beckman Postdoctoral Fellowship (2016); National Defense Science and Engineering Graduate Fellowship (2011); NSF Graduate Research Fellowship (2011).

The identification and characterization of transient intermediates is crucial for developing detailed molecular-level knowledge of chemical reaction mechanisms – insight that is required to fully understand important biological processes like photosynthesis, energy storage and transfer, and for the rational development of novel synthetic catalysts. However, key reaction intermediates and their dynamics are often too short-lived or technically challenging to capture and interrogate directly with current methods. Next-generation methods are required to isolate and probe elusive reaction intermediates and transition-state species with atomistic detail.

Our research program seeks to develop novel experimental techniques which will allow for the capture and direct interrogation of reaction intermediates by combining the high sensitivity and selectivity of mass spectrometry, the high-frequency resolution of gas-phase ion spectroscopies, and the time resolution of ultrafast spectroscopies in a single experiment.

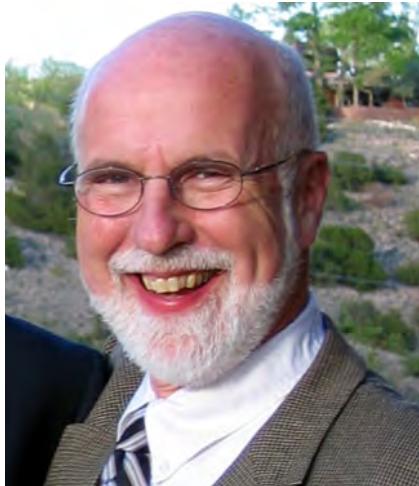
The versatility of mass spectrometric techniques allows for the careful control and manipulation of the chemical system of interest in a composition-selective manner, allowing for the isolation of well-defined chemical architectures. Cryogenic cooling (10 K) of these isolated systems in an ion trap allows us to obtain highly resolved optical spectra, yielding unambiguous structural identification. The time evolution of the spectroscopic transitions with ultrafast resolution will help us characterize the time-evolving shape of the reactive potential energy surface (PES). This data will provide the basis for clear mechanistic interpretation of fast chemical reactions and how the surrounding chemical environment actively dictates the reaction dynamics and underlying shape of the PES.

Specifically, we are interested in studying catalytic processes driven by proton-coupled electron transfer (PCET), which are ubiquitous throughout chemistry and biology. Our focus will include two forefront problems where clear mechanistic details are vitally needed: (1) The role of tyrosine and tryptophan in biological PCET, in particular, the nature and dynamics of TyrOH^+ and TrpNH^+ radical cation species which are proposed key intermediates across numerous catalytic proton transport pathways. (2) Capturing intermediates generated during the activation of small molecules by organometallic catalysts, specifically, how solvent waters around the active site and ligand composition in water oxidation catalysts drive the formation of the proposed high-valent metal-oxo intermediates.



Selected Publications

- L. Chen; E.L. Sibert III, J.A. Fournier. "Unraveling the Vibrational Spectral Signatures of a Dislocated H atom in Model Proton Coupled Electron Transfer Dyad Systems." *J. Phys. Chem. A* 2023, accepted.
- L. Chen, Z. Ma, J.A. Fournier. "Origins of the Diffuse Shared Proton Vibrational Signatures in Proton-Coupled Electron Transfer Model Dyad Complexes." *J. Chem. Phys.* 2022, **157**, 154308. Editor's Pick article.
- J.L.S. Dean, J.A. Fournier. "Vibrational Dynamics of the Intramolecular H-Bond in Acetylacetone Investigated with Transient and 2D IR Spectroscopy." *J. Phys. Chem. B* 2022, **126**, 3551.
- L. Chen, J.L.S. Dean, J.A. Fournier. "Time-Domain Vibrational Action Spectroscopy of Cryogenically Cooled, Messenger-Tagged Ions Using Ultrafast IR Pulses." *J. Phys. Chem. A* 2021, **125**, 10235.
- L. Chen, J.A. Fournier. "Probing Hydrogen-Bonding Interactions within Phenol-Benzimidazole Proton-Coupled Electron Transfer Model Complexes with Cryogenic Ion Vibrational Spectroscopy." *J. Phys. Chem. A* 2021, **125**, 9288.



PROFESSOR

Analytical, Organic, and Biophysical Chemistry;
Joint with Internal Medicine and Immunology

Michael L. Gross

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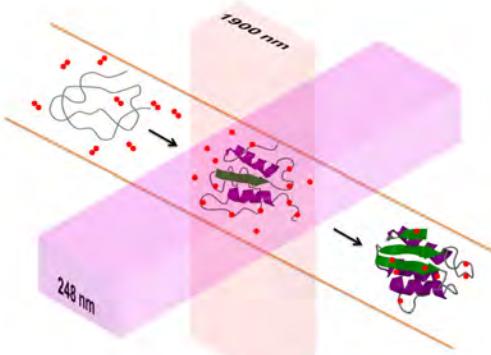
mgross@wustl.edu

Postdoctoral, Purdue University (1967-8); Postdoctoral, U. of Penn. (1966-7); Ph.D., University of Minnesota (1966); B.A., (Cum Laude) St. John's University, Minnesota (1962).

Wolfgang Paul Lectureship, German and Polish MS Society (2012), Honorary Lifetime Membership, Mass Spectrometry Society of Japan, Freiser Lectureship, Purdue University (2008), J.J. Thomson Medal for Service to Int'l MS (2006), Sommer Award, Department of Chemistry, University of Nebraska (2004); Midwest Award for Achievements in Chemistry, ACS (2002); Excellence in Mentoring Award, WU Graduate Senate (2001-4); Field and Franklin Award, ACS (1999).

Our main goal is to develop mass spectrometric methods to understand interactions between proteins and ligands, a general approach known as “protein footprinting.” To this end, we introduced PLIMSTEX (Protein Ligand Interaction by Mass Spectrometry, Titration and H/D Exchange) whereby we use hydrogen/deuterium exchange as a reporter for the titration of a protein with a ligand. The titration yields the affinity of binding, and with digestion of the protein and further MS analysis, the site and order of binding can be determined.

A complementary approach developed in our laboratory, fast photochemical oxidation of proteins (FPOP), makes use of reactive species ($\cdot\text{OH}$, $\cdot\text{OSO}^{3-}$, $\cdot\text{I}$) that are formed by a pulsed laser (KrF) in tens of nanoseconds in the presence of proteins. The radicals react with the amino-acid side chains to footprint them (i.e., to report whether the side chain is solvent-accessible or buried, part of an interface, or protected by an interaction with ligand). By controlling the radical concentration with a scavenger, the lifetime of the radicals can be limited to $\sim 1 \mu\text{s}$, thus affording a method that produces a “snapshot” of a protein.



We utilize the speed of this footprinting in a study whereby another laser (1900 nm) is used to produce a “temperature jump” in a flowing proteins solution followed by the FPOP laser (248 nm) that produces $\cdot\text{OH}$ and footprints the protein during the time it folds or unfolds. In the accompanying scheme, one can see the unfolded protein in the presence of H_2O_2 . As the solution flows past the first laser beam, the temperature increases rapidly, causing this protein to fold. The second laser produces $\cdot\text{OH}$ whose reactions report on the status of the folding protein.

Another research interest is Fourier transform MS. We design new cells to overcome problems of detecting high-mass biomolecules, a development that will be important in

proteomics and therapeutic protein development. We are also interested in studying high mass protein assemblies that we introduce in the gas phase by native (non-denaturing) electrospray ionization and study them by using, for example, electron-capture dissociation.

The laboratory is one of seven nationwide that is supported by the National Institutes of General Medicine of the NIH to develop biotechnology based on mass spectrometry. Under the aegis of this center, students do basic research, participate in collaborative research in protein structural problems, and learn both bottom-up and top-down proteomics. The research groups works with a variety of high-performance mass spectrometers including FTICRs, Q-ToF, and orbitraps and with HPLCs.

Selected Publications

- Protein Footprinting and X-ray Crystallography Reveal the Interaction of PD-L1 and a Macrocyclic Peptide, Ben Niu, Todd C. Appleby, Ruth Wang, Mariya Morar, Johannes Voight, Armando G. Villaseñor, Sheila Clancy, Sarah Wise, Jean-Philippe Belzile, Giuseppe Papalia, Melanie Wong, Katherine M. Brendza, Latesh Lad, and Michael L. Gross, *Biochemistry*, 59, 541-551 (2020). PMC7485629
- The Application of Fluorine-Containing Reagents in Structural Proteomics, Ming Cheng, Chunyang Guo, and Michael L. Gross, *Angewandte Chemie-International Edition*, 59, 5880-5889 (2020). Also published in German: Fluorierte Reagenzien in der Strukturproteomik, *Angew. Chemie*, 132, 5932-5942 (2020). PMC7485648
- The Cap-Snatching SFTSV Endonuclease Domain is an Antiviral Target, Wenjie Wang, Woo Jin Shin, Bojie Zhang, Younho Choi, Ji Seung Yoo, Maxwell I. Zimmerman, Thomas E. Frederick, Gregory R. Bowman, Michael L. Gross, Daisy W. Leung, Jae U. Jung, Gaya K. Amarasinghe, *Cell Reports*, 30, 153-163.e5 (2020). PMC7214099
- Mass Spectrometry-Based Protein Footprinting for Higher Order Structure Analysis: Fundamentals and Applications, Xiaoran Roger Liu, Mengru Mira Zhang, and Michael L. Gross, *Chemical Reviews*, 120, 10, 4355-4454 (2020).. Revising High Resolution Crystal Structure of Phormidui



**PROFESSOR
VICE DEAN OF GRADUATE EDUCATION**

Inorganic/Materials Chemistry

Sophia Hayes

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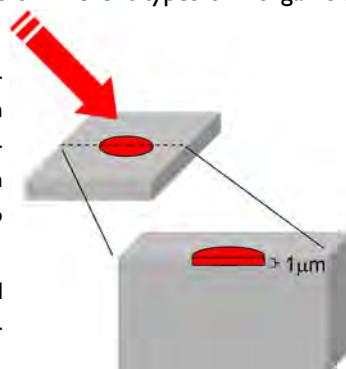
Postdoctoral Fellow, University of Dortmund (2001); LLNL and U.C.Berkeley (1998-2000); Ph.D., U.C. Santa Barbara (1999); B.S., U.C. Berkeley (1990).

American Physical Society, "5 σ Physicist" Award (2020); St. Louis Award, American Chemical Society (2015); NSF CAREER Award (2003); Alexander von Humboldt Postdoctoral Fellow (2001); Directorate Postdoctoral Fellow, LLNL (1998-2000).

The goal of Professor Hayes' research group is a basic understanding of the structure and properties of different types of inorganic systems, including semiconductors and other optically and electronically active materials.

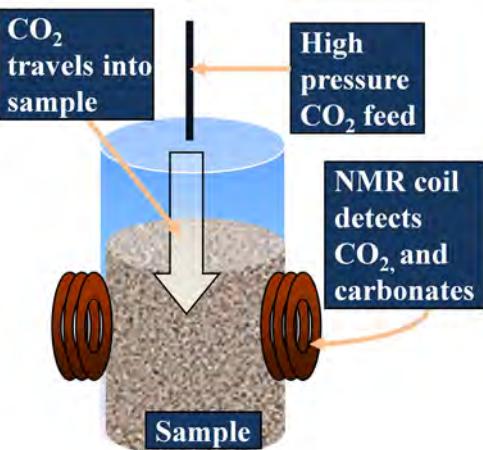
Optically-pumped NMR: Development and application of optically-pumped (OPNMR) and optically-detected (ODNMR) NMR of bulk semiconductors and quantum wells to gain insight into the interplay between photogeneration of conduction electrons, electron spin polarization, and resulting nuclear spin polarization. Surface and interface structures, as well as characterization of defects in the materials and spin diffusion processes that can polarize distant spins are being studied. These research foci have particular relevance to solar energy materials and LED applications.

Computation of NMR tensors and spectra prediction: Creation of an NMR library of spin-1/2 and quadrupolar tensors through The Materials Project, computing NMR tensors from crystal structures of dominantly inorganic compounds. Density functional theory calculations of NMR tensors in CASTEP and VASP.



NMR crystallography: using the tensor catalogue, we work on refinements of atomic coordinates for materials where the NMR and X-ray diffraction lead to slightly different predictions of structure. NMR can be used to refine atomic coordinates, especially for species such H-atoms.

Carbon capture & sequestration: NMR characterization of CO₂ (and CH₄) chemisorption and physisorption in materials tailored for greenhouse gas removal. Some studies are by *in situ* high-pressure high-temperature CO₂ NMR studies of gas, liquid, and supercritical CO₂ in the presence of geological (porous) rock samples and in materials designed for the capture of CO₂ or other gaseous materials (such as methane, and acid gases including SO_x, NO_x).



Solid-state NMR studies on quadrupolar (nuclear spin, I > 1/2) systems: diverse nuclei studied, including many Group III inorganic molecular clusters that are deposited as thin metal oxide films used as dielectrics in semiconductor devices. The focus has been predominantly 27Al, 69Ga, 71Ga, 51V measurements and modeling of the quadrupolar lineshapes.

Topochemistry: solid-state single crystal-to-single crystal photo-cycloaddition reactions can be monitored via solid-state NMR, given our unique hardware for incorporating laser irradiation at the sample space. NMR was able to determine reaction kinetics of cinnamic acid to truxillic acid conversions, and examine additional derivatives.

Selected Publications

- M.E. West, E.L. Sesti, M.M. Willmering, D.D. Wheeler, Z. Ma, L. Zayd, S.E. Hayes*, "Describing Angular Momentum Conventions in Circularly Polarized Optically Pumped NMR (OPNMR) in GaAs and CdTe" *J. Magn. Reson.*, **327**, 106980 (2021).
- H. Sun, S. Dwarkanath, H. Ling, X. Qu, K. Persson, S. Hayes*, "Enabling Materials Informatics for ²⁹Si Solid-state NMR of Crystalline Materials", (*Nature Publishing Group*) *npj Computational Materials*, **6**, 53 (2020).
- J. Cui, D. Olmsted, A.K. Mehta, M. Asta, S.E. Hayes*, "NMR Crystallography: Evaluation of Hydrogen Positions in Hydromagnesite by ¹³C{¹H} REDOR Solid-State NMR and Density Functional Theory Calculation of Chemical Shielding Tensors", *Angew. Chem. Int. Ed.*, **58**, 4210-4216 (2019).
- J. Cui, M.G. Kast, B.A. Hammann, Y. Afriyie, K.N. Woods, P.N. Plassmeyer, C.K. Perkins, K. Cory, Z.L. Ma, D.A. Keszler, C.J. Page, S.W. Boettcher, S.E. Hayes*, "Aluminum Oxide Thin Films from Aqueous Solutions: Insights from Solid-State NMR and Dielectric Response", *Chem. Mater.*, **30**, 7456-63 (2018).
- C.-H. Chen, D. Shimon, J.J. Lee, F. Mentink-Vigier, I. Hung, C. Sievers, C. Jones, S.E. Hayes*, "The 'Missing' Bicarbonate in CO₂ Chemisorption Reactions on Solid Amine Sorbents", *J. Am. Chem. Soc.*, **140**, 8648-8651 (2018).

ASSISTANT PROFESSOR

Open quantum systems, quantum computing, algorithms, quantum dynamics, electronic structure theory, reduced density matrices, transition metal chemistry

Kade Head-Marsden

Postdoctoral Fellow, Harvard University (2019-22); Ph.D., University of Chicago (2019); B.S., McGill University (2014)



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Physical Sciences Fellowship, Univ. of Chicago (2019); College Teaching Certificate, Univ. of Chicago (2019); Nathan Sugarman Teaching Award for General Chemistry, Univ. of Chicago (2015); Hypercube Scholar, McGill Univ. (2014); NSERC Undergraduate Research Award Theoretical chemistry McGill Univ. (2013); Thomlinson Teaching Award, McGill Univ. (2013).

The Head-Marsden Group seeks to elucidate electronic structure properties and open quantum system dynamics relevant in emerging quantum materials and technologies. Our research emphasizes on classical method development, alongside algorithm development for use on noisy-intermediate scale quantum computers. With these methods and algorithms, we hope to make predictions for correlated molecular systems undergoing complex environmental interactions with applications in chemistry, physics, and materials science.

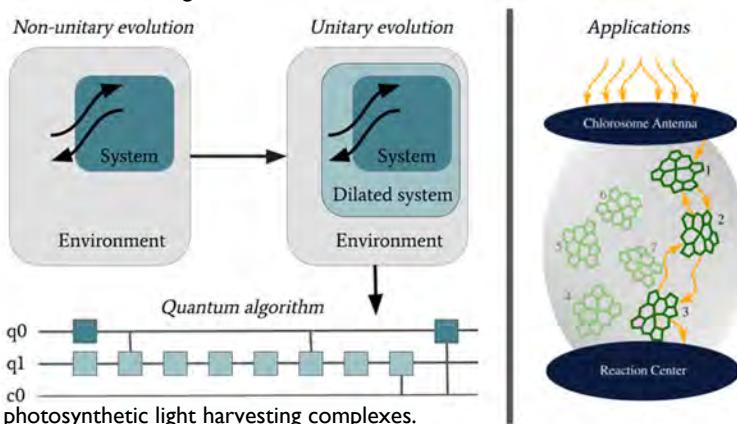
Contemporary problems in materials science and chemistry require theoretical and computational methods that accurately and efficiently capture quantum behavior. Important phenomena including exciton transport and decoherence dynamics in quantum systems are frequently driven by interactions with an external environment. The field of open quantum systems provides a lens to consider such environmentally driven dynamical processes. Our research focuses on developing and applying methods in open quantum systems, quantum information, and electronic structure to provide a holistic perspective on molecular, material, and condensed matter systems.

Key areas of research include:

- Classical method development for the treatment of complex environmentally driven dynamics in open quantum systems
- Quantum algorithm development for chemical applications with an emphasis on time-evolving electronic structure
- Open quantum system methods applied to quantum hardware characterization
- Electronic structure characterization of correlated molecular and material systems

Figure (Left): Our research consists of classical method development for open quantum system dynamics, or non-unitary dynamical evolution. To perform comparable evolution on a quantum computer, we can map this framework into a unitary evolution that can then be implemented as a gate-based algorithm on noisy intermediate-scale quantum devices.

Figure (Right) Through these classical methods and quantum algorithms we can consider the time evolution of important quantum systems, such as photosynthetic light harvesting complexes.



Selected Publications

- A.W. Schlimgen, K. Head-Marsden, L.M. Sager, P. Narang, and D.A. Mazziotti, "Quantum Simulation of Open Quantum Systems Using a Unitary Decomposition of Operators", arXiv:2106.12588 (2021)." to "A.W. Schlimgen, K. Head-Marsden, L.M. Sager-Smith, P. Narang, and D.A. Mazziotti, "Quantum Simulation of Open Quantum Systems Using a Unitary Decomposition of Operators", Phys. Rev. Lett. 127 (27), 270503 (2021).".
- K. Head-Marsden, S. Krastanov, D.A. Mazziotti, P. Narang, "Capturing Non-Markovian Dynamics on Near-Term Quantum Computers", Phys. Rev. Res., 3, 013182 (2021).
- K. Head-Marsden and D.A. Mazziotti, "Ensemble of Lindblad's Trajectories for Non-Markovian Dynamics", Phys. Rev. A, 99, 022109 (2019).
- K. Head-Marsden and D.A. Mazziotti, "Active Space Pair Two-Electron Reduced Density Matrix Theory for Strong Correlation", J. Phys. Chem. A, 124, 4848-54 (2020).
- A.W. Schlimgen, K. Head-Marsden, L.M. Sager, P. Narang, and D.A. Mazziotti, "Quantum Simulation of Open Quantum Systems Using a Unitary Decomposition of Operators", arXiv:2106.12588 (2021).



Chemical Biology Jennifer Heemstra

Ph.d, University Of Illinois, Urbana-Champaign; BS., University Of California, Irvine



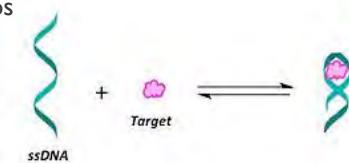
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ACS WCC Rising Star Award (2021); UPenn Women in Chemistry Leadership in Science Award (2020); Scialog Fellow, Chemical Machinery of the Cell (2018); W.W. Epstein Outstanding Educator Award (2016); NSF CAREER Award (2016); Cottrell Scholar Award (2015); Myriad Award of Research Excellence (2015); University of Utah College of Science Professorship (2014); NSF MRSEC Young Investigator Lectureship (2013); Army Research Office Young Investigator Award (2011)

Nucleic acids are exquisitely adept at molecular recognition and self-assembly, enabling them to direct numerous key processes that make life possible. These capabilities have been fine-tuned by billions of years of evolution and have been harnessed in the laboratory to enable the use of DNA and RNA for applications beyond their canonical biological roles. The common thread that is woven throughout the research projects in the Heemstra Lab is the utilization of nucleic acid molecular recognition and self-assembly to generate functional architectures for biosensing and bioimaging.

Small Molecule Detection and Sequestration

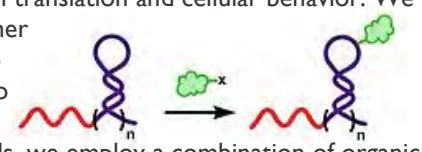
Nucleic acid aptamers offer a promising alternative to antibodies for a wide range of biosensing applications. We have demonstrated the use of a split aptamer to transduce a small molecule signal into the output of a DNA ligation event. If present in solution, the target molecule directs assembly of the split aptamer, bringing DNA-appended reactive groups into close proximity and thus promoting a chemical ligation. We have demonstrated that this enables the sensitive and selective detection of drug molecules in an enzyme-linked format, which is the current gold standard in clinical diagnostics. We have also addressed an overarching challenge in this field – the dearth of split aptamer recognition elements – by developing a reliable method for the engineering of aptamers into split aptamers.



Moving beyond detection to characterization, we seek to address the challenging task of measuring small molecule enantiopurity, as this is a key factor in the synthesis of pharmaceutical intermediates and other high-value chemicals. Enantiopurity can be measured by chiral chromatographic methods, but this process is limited to a few thousand samples per day. Utilizing the principle of reciprocal chiral substrate selectivity, we have generated enantiomeric DNA biosensors capable of measuring small molecule enantiopurity with a direct fluorescence output, which provides significantly increased throughput. We envision application of this method to optimize stereoselectivity in reactions using either chemical or biological catalysts.

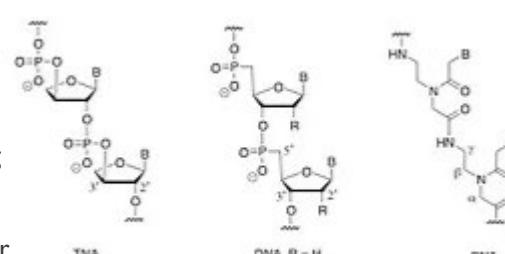
Post-Transcriptional Modification

In Nature, information typically flows from DNA to RNA to protein, telling the cell what to do, where to do it, and how often. RNA serves as the “messenger” of this information, and its location in the cell is pivotal to cellular function. As such, being able to track RNAs in real time while they move around in the cell would be incredibly valuable in elucidating the interworking of protein translation and cellular behavior. We are also now learning that RNA can be chemically modified and “edited” after transcription, adding another complex layer of information and eliciting profound changes in overall cellular function. Given the importance of RNA localization and editing, we’re interested in developing new chemical and biological tools to track RNA in living cells. We’re also creating new methods to study RNA editing and even insert these changes in new locations for synthetic biology and genetic engineering applications. To achieve these goals, we employ a combination of organic synthesis, molecular biology, and directed evolution methods to engineer new nucleic acid and protein tools, and we evaluate these constructs in a variety of chemical, biological, and cellular assays for *in vitro* and *in vivo* applications.



Unnatural Nucleic Acids

Peptide nucleic acid (PNA) is a nucleic acid analog in which the phosphodiester backbone is replaced with a peptide-like aminoethylglycine unit. PNA shows great potential for use *in vivo* due to its higher affinity and selectivity for native nucleic acids as well as its increased resistance to degradation by nucleases and proteases. In order to expand the role of PNA in these applications, we have investigated the impact of backbone modification on binding with DNA and RNA. We are also exploring the ability of PNA functionalization to drive self-assembly into micellar architectures capable of acting as programmable materials.



Threose Nucleic Acids (TNA) are variants of naturally-occurring nucleic acids that differ in the lengths and connectivity of the sugar-phosphate backbone. TNA is capable of undergoing transcription, reverse-transcription and participating in Watson-Crick base pairing while providing increased resistance to nuclease degradation. The unique properties of TNA allow for its use as an alternative genetic information system and as a nuclease resistant biopolymer capable of adopting secondary structure. In our research, we have examined the transcription of modified TNA bases from DNA templates and have investigated the fundamental properties that influence TNA-DNA hybridization. In addition, we have employed a directed evolution strategy to select for a high-affinity, nuclease-resistant TNA aptamer capable of binding small molecule toxins.



PROFESSOR

Physical/Biophysical Chemistry

Dewey Holten

National Needs Postdoctoral Associate, Washington State University (1977-80); Ph.D., University of Washington (1976); B.A., Washington University (1973).

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Professor Holten's research interests include the initial reactions of photosynthesis and photophysical studies of tetrapyrrole chromophores and arrays. The goals of his lab's photosynthesis research are to achieve a molecular-level understanding of charge separation in the bacterial reaction center and design of mutants that endow the reaction center with properties not realized in nature. The goals of the tetrapyrrole research are to elucidate the electronic properties of natural and synthetic tetrapyrroles, address fundamental questions in energy and electron transfer, and tailor systems for a range of applications.

In the reaction center pigment-protein complex, light energy is converted into chemical potential energy by a series of fast electron transfers across the membrane from the photoexcited bacteriochlorophyll special dimer along a chain of electron acceptors on the photoactive A-branch with a quantum yield of ~1. His lab is studying mutants to (1) modulate the rate constants, yields and mechanisms of charge separation versus recombination at each step on both A and B branches, and (2) give electron transfer fully down the normally inactive B branch. The studies of tetrapyrrole chromophores (porphyrin, chlorin, bacteriochlorin) are aimed at elucidating the interplay between molecular composition, electronic structure, and photophysical properties. These properties include absorption and emission spectra and the rate constants and yields of the singlet excited-state decay pathways (fluorescence, internal conversion, inter-system crossing). Studies of multichromophore arrays probe fundamental aspects of energy and electron transfer including the potential effects of coherence phenomena. The collective studies provide insights and design principles that for constructing chromophores and arrays for use in solar-energy and life-sciences research.

Selected Publications

- Tailoring Panchromatic Absorption and Excited-State Dynamics of Tetrapyrrole-Chromophore (Bodipy, Rylene) Arrays. The Interplay of Orbital Mixing and Configuration Interaction, A. K. Mandal, J. R. Diers, D. M. Niedzwiedzki, G. Hu, R. Liu, E. J. Alexy, J. S. Lindsey, D. F. Bocian, and D. Holten, *J. Am. Chem. Soc.* 2017, 139, 17547-17564.
- Origin of Panchromaticity in Multichromophore-Tetrapyrrole Arrays, J. M. Yuen, J. R. Diers, E. J. Alexy, A. Roy, A. K. Mandal, H. S. Kang, D. M. Niedzwiedzki, C. Kirmaier, J. S. Lindsey, D. F. B, and D. Holten , *J. Phys. Chem. A* 2018, 122, 7181-7201.122, 7181-7201.
- Annulated Bacteriochlorins for Near-Infrared Photophysical Studies, H. Fujita, H. Jing, M. Krayer, S. Allu, G. Veeraraghavaiah, Z. Wu, J. Jiang, J. R. Diers, N. C. M. Magdaong, A. K. Mandal, A. Roy, D. M. Niedzwiedzki, C. Kirmaier, D. F. Bocian, D. Holten and J. S. Lindsey, *New Journal of Chemistry* 2019, 3, 7209-7232.
- Switching Sides - Re-Engineered Primary Charge Separation in the Bacterial Photosynthetic Reaction Center, P. D. Laible, D. K. Hanson, J C. Burhmaster, G. A. Tira, K. M. Faries, D. Holten, and C. Kirmaier, *Proc. Nat Acad. Sci. U.S.A.* 2020, 117, 865-871.
- Photophysical Properties and Electronic Structure of Zinc(II) Porphyrins Bearing Zero to Four meso-Phenyl Substituents – Zinc Porphine to Zinc Tetraphenylporphyrin (ZnTPP), N. C. M. Magdaong, M. Taniguchi, J. R. Diers, D. M. Niedzwiedzki, C. Kirmaier, J. S. Lindsey, D. F. Bocian, and D. Holten, *J. Phys. Chem. A* 2020, 124, 7777-7794.
- In Situ, Protein-Mediated Generation of a Photochemically Active Chlorophyll Analog in a Mutant Bacterial Photosynthetic Reaction Center, N. C. M. Magdaong, J. C. Buhrmaster, K. M. Faries, H. Liu, G. A. Tira, J. S. Lindsey, D. K. Hanson, D. Holten, P. D. Laible, and C. Kirmaier, *Biochemistry* 2021, 60, 1260-1275.
- Perspective on the Redox Properties of Tetrapyrrole Macrocycles, J. R. Diers, C. Kirmaier, M. Taniguchi, J. S. Lindsey, D. F. Bocian, and D. Holten, *Phys. Chem. Chem. Phys.* 2021, 23, 19130–19140.
- Probing the Effects of Electronic-Vibrational Resonance on the Rate of Excited-State Energy Transfer in Bacteriochlorin Dyads, N. C. M. Magdaong, H. Jing, J. R. Diers, C. Kirmaier, J. S. Lindsey, D. F. Bocian, and D. Holten, *J. Phys. Chem. Lett.* 2022, 13, 7906-7910. 3
- High Yield of B-side Electron Transfer at 77 K in the Photosynthetic Reaction Center Protein from Rhodobacter sphaeroides, N.C. M. Magdaong, K. M. Faries, J. C. Buhrmaster, G. A. Tira, R. M. Wyllie, C. E. Kohout, D. K. Hanson, P. D. Laible, D. Holten, and C. Kirmaier, *J. Phys. Chem. B* 2022, 126, 8940-8956.
- Balancing Panchromatic Absorption and Multistep Charge Separation in a Compact Molecular Architecture, A. Roy, N. C. M. Magdaong, H. Jing, J. Rong, J. R. Diers, H. S. Kang, D. M. Niedzwiedzki, M. Taniguchi, C. Kirmaier, J. S. Lindsey, D. F. Bocian, and D. Holten, *J. Phys. Chem. A* 2022, 126, 9352-9365.

ASSISTANT PROFESSOR



Biochemistry and Chemical Biology Meredith Jackrel

Postdoctoral Fellow, Perelman School of Medicine at the University of Pennsylvania (2010-2017); Ph.D., Yale University (2010); B.S., The College of New Jersey (2004).

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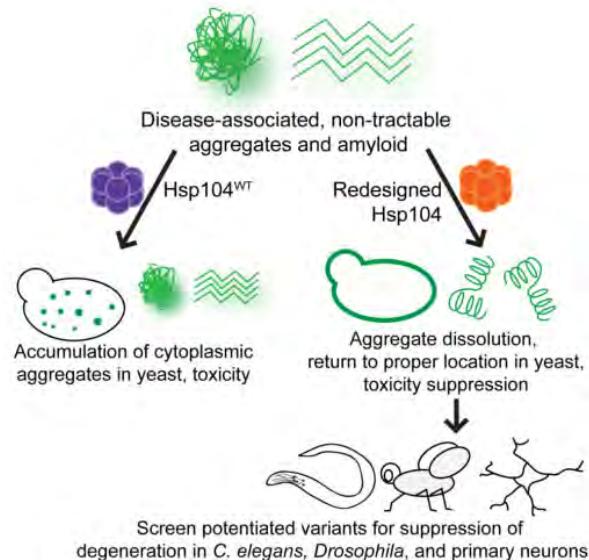
My interests include protein folding, misfolding, biomolecular condensates, and neurodegenerative disease; protein chaperones; and protein engineering.

We use protein engineering and directed evolution to develop specialized molecular machines to reverse the protein misfolding implicated in human disease. In neurodegenerative diseases such as Parkinson's disease (PD), amyotrophic lateral sclerosis (ALS), and Alzheimer's disease (AD), specific proteins misfold to take on the amyloid conformation. While traditionally viewed as an intractable and highly toxic protein conformation, amyloid is not always toxic. In fact, yeast employ amyloid for beneficial purposes and have evolved pathways to construct and disassemble amyloid. We are interested in reformulating this pathway and applying it to target human disease. The protein controlling this pathway in yeast is Hsp104, and in yeast Hsp104 disaggregates proteins from amyloid fibrils, pre-amyloid oligomers, and disordered aggregates. The amyloid fold is highly conserved, suggesting that Hsp104 might disaggregate amyloids comprised of other proteins. However, Hsp104 has only limited activity against amyloid fibrils comprised of proteins such as α -synuclein and A β (implicated in PD and AD, respectively). Thus, we aim to enhance Hsp104 activity and re-engineer Hsp104 substrate specificity. We use yeast as a model system because Hsp104 is present in yeast and powerful genetic tools are available to manipulate yeast. Also, expression of disease-associated substrates in yeast results in the accumulation of aggregated proteins that confer toxicity, which recapitulates their pathologies in human disease and has empowered the identification of genetic risk factors in humans. Using these models, we have developed a series of Hsp104 variants that potently disassemble TDP-43, FUS, and α -synuclein aggregates and amyloids that are implicated in ALS and PD. The variants we have developed suppress the toxicity of these misfolded proteins and also clear preformed aggregates, allowing the substrates to return to their proper localization. Certain variants potently suppress neurodegeneration in a *C. elegans* PD model and reverse aggregation in mammalian fibroblasts. In addition to their possible therapeutic applications, these variants might be employed as probes to study the underpinnings of protein-misfolding disorders.

Our first generation variants are highly promising, but require further tuning to improve their characteristics. Thus we employ protein engineering and directed evolution to tune the activity of Hsp104 and other chaperones in order to develop variants with desired properties. We predict that just as numerous other proteins have evolved from generalists to specialists over many years of evolution, we can evolve Hsp104 from a generalist to a specialized molecular machine. Recently, several disaggregases were discovered in humans, and we are also working to better understand their mechanisms and how they might be targeted therapeutically. Protein misfolding is implicated in numerous other diseases. Thus we are interested in developing yeast models for these disorders and applying disaggregases to counter the misfolding of these substrates. For instance, we have demonstrated that biofilm protein amyloidogenesis can be modeled in yeast, and provides a tractable platform for studying biofilm formation and modulation. Finally, we are interested in using pure protein biochemistry and structural biology to better understand disaggregase structure and mechanism. Amyloid is incredibly stable, thus we seek to understand how disaggregases disassemble amyloid.

Selected Publications

- M.K. Howard, K.R. Miller, B.S. Sohn, J.J. Ryan, A. Xu, and M.E. Jackrel* (2023). Probing the drivers of *Staphylococcus aureus* biofilm protein amyloidogenesis and disrupting biofilms with engineered protein disaggregases. *mBio*.
- M.L. Sprunger, K. Lee, B.S. Sohn, and M.E. Jackrel* (2022). Molecular determinants and modifiers of Matrin-3 toxicity, condensate dynamics, and droplet morphology. *iScience*. 25(3):103900.
- M.L. Sprunger and M.E. Jackrel*, "Prion-like Proteins in Phase Separation and Their Link to Disease." *Biomolecules*, 11, 1014 (2021).
- J.J. Ryan, A. Bao, B. Bell, C. Ling, M.E. Jackrel*, "Drivers of Hsp104 Potentiation Revealed by Scanning Mutagenesis of the Middle Domain." *Protein Science*, 30, 1667-1685 (2021).
- M.K. Howard, B.S. Sohn, J. von Borcke, A. Xu, and M.E. Jackrel*, "Functional Analysis of Proposed Substrate-binding Residues of Hsp104." *PLoS ONE*, 15, e0230198 (2020).
- A. Tariq, J. Lin, M.E. Jackrel, C.D. Hesketh, P.J. Carman, K.L. Mack, R. Weitzman, C. Gambogi, O.A. Hernandez Murillo, E.A. Sweeny, E. Gurpinar, A.L. Yokom, S.N. Gates, K. Yee, S. Sudesh, J. Stillman, A.N. Rizo, D.R. Southworth, and J. Shorter*. "Mining Disaggregase Sequence Space to Safely Counter TDP-43, FUS, and Alpha-synuclein Proteotoxicity." *Cell Rep.*, 28, 2080–2095 (2019).
- M.L. Sprunger and M.E. Jackrel*. "Quality Control in the ER: Misfolded Prohormones Get a Checkup." *Mol. Cell*, 75, 415-416 (2019).





ASSOCIATE PROFESSOR

Supramolecular chemistry, Polymer chemistry, Solid-state chemistry, 3D printing polymer design, Porous organic frameworks, Carbohydrate recognition, Water purifications, Chemical separations, Hydrogel, Stimuli-responsive systems Chemistry

Chenfeng Ke

*Postdoctoral fellow, Northwestern University
Newton fellow, University of Bristol
PhD and BS, Nankai University*

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The Ke research group aims to mimic the design principles of natural materials and to develop the next generation of artificial materials that possess sophisticated molecular features and hierarchy, multifunctionality, and chemical/mechanical stimuli-responsiveness. My research program is subdivided into three major thrusts:

Thrust 1 centers on the integration of three-dimensional (3D)-printing techniques with molecular design to develop stimuli-responsive 3D-printing hydrogels for soft robotics and tissue regenerations.

Thrust 2 weds the concepts of supramolecular self-assembly with crystal engineering to design a new family of porous organic materials with unique elastic properties. These light-weight, durable, and porous scaffolds can be used for water purification and petrochemical separations.

Thrust 3 aims to develop a Ca²⁺-dependent carbohydrate binding protein analog (synthetic C-type lectins) to bind mono- and oligo-

Appointments

Associate Professor, 2024, Department of Chemistry, Washington University in St. Louis
Assistant and Associate Professor, 2015-2023, Department of Chemistry, Dartmouth College

Selected Awards

Scholarly Innovation and Advancement Award, Dartmouth College, 2023
Top 10% of reviewers for Angewandte Chemie for year 2022, 2023
Susan and Gib Myers 1964 Faculty Fellowship, Dartmouth College, 2022
Karen E. Wetterhahn Memorial Award for Distinguished Creative or Scholarly Achievement, Dartmouth College, 2022
American Chemical Society PMSE Young Investigator Award, 2021
Cram Lehn Pedersen Prize in Supramolecular Chemistry, 2020
Beckman Young Investigator Award, 2019, the Beckman Foundation



PROFESSOR

Physical & Materials Chemistry

Richard A. Loomis

NRC Postdoctoral Fellow, NIST-University of Colorado (1996-8); Ph.D., University of Pennsylvania (1995); B.S., Dickinson College (1989).

Awards: ACS St. Louis Award (2020); WU A&S Dean's Community Response Award (2020); WU CSAS Faculty Award for Teaching (2000, 2004, 2008, 2019); WU David Hadas Teaching Award in A&S (2012); WU FCC Outstanding Professor of the Year (2010); WU GSS Outstanding Faculty Mentor Award (2008); NSF CAREER Award (2004); David & Lucile Packard Fellowship in Science and Engineering (2001); Research Corporation, Research Innovation Award (1999); Camille & Henry Dreyfus, New Faculty Award (1998).

Current thrusts include the spectroscopic characterization of charge carrier dynamics within semiconductor nanostructures, bimolecular interactions, and the coherent control of chemical dynamics. The experiments utilize an array of tools, including steady-state and time-resolved single-molecule microscopy, transient-absorption spectroscopy, nanosecond and state-of-the-art femtosecond lasers, ultrashort pulse shaping, mass spectrometry and ion imaging, and absorption, fluorescence, and non-linear spectroscopy.

Charge and Exciton Dynamics within Semiconductor Nanostructures. A number of spectroscopic techniques are utilized to determine how shape affects the optical properties of semiconductor quantum nanostructures. Specifically, we, in collaboration with the group of Professor Buhro, are investigating the dependence of band gap energies on the diameter of semiconductor quantum wires. These quantum wires are ideal for studying the two-dimensional quantum confinement of excitons and propagation of charge carriers over long distances since they can be synthesized with diameters as small as 3.5 nm and lengths on the order of tens of microns. We are now using a confocal microscope coupled with ultrafast lasers to directly measure the excitonic dynamics within individual nanowires as a function of temperature, exciton energy, and chemical composition of the nano-material. Some of these quantum wires exhibit photoluminescence intensity blinking spanning the entire lengths of quantum wires. We continue to investigate the origins of this blinking in these unique quantum-mechanical systems.

Bimolecular Interactions and Reaction Dynamics. Frequency and time-resolved laser spectroscopy and time-of-flight ion imaging methods are implemented to accurately characterize inter-molecular potential energy surfaces and the dynamics that occur on these surfaces. Two moieties are first stabilized in a weakly bound complex by cooling the species in a supersonic expansion. By cooling the complexes to specific temperatures, we are able to stabilize the complexes with preferred orientations between the constituents. The $\text{He} \cdots \text{ICl}(X,v=0)$ complex, for instance, is found to have a T-shaped orientation at $T \sim 5$ K and at lower temperatures, $T \sim 0.5$ K, the complexes have preferred linear geometries. These complexes serve as launching pads for investigating the photo-induced dynamics that occur from these initial orientations.

Coherent Control of Chemical Dynamics. Ultrashort laser pulses are used to initiate and monitor the dynamics of molecules that can follow competing pathways. Furthermore, the properties of the excitation pulse are manipulated to quantum mechanically control the yields of the different product channels. The coherent control of biomolecular reactions is also being pursued. Two reactants are stabilized in a non-reactive complex. A laser promotes the reactants above the barrier for reaction. **The probability for reaction is then controlled by steering the reactants to specific intermolecular orientations and energies.**

Selected Publications

- J. Chen, W.M. Sanderson, and R.A. Loomis*, “Effects of Competing Pathways on Carrier Relaxation in Semiconductor Quantum Wires”, submitted to *ACS Nano* (2021).
- C. Makarem, J. Wei, R.A. Loomis*, and J.P. Darr*, “Vibrational Predissociation versus Intramolecular Vibrational Energy Redistribution (IVR): IVR Identified in $\text{Ar} \cdots \text{I}_2(B,v)$ Using Velocity-Map Imaging”, submitted to *Phys. Chem. Chem. Phys.* (2021).
- W.M. Sanderson, J. Schrier, and R.A. Loomis*, “Photo-induced State Shifting in 1D Semiconductor Quantum Wires”, *J. Phys. Chem. C*, **124**, 16702-13 (2020).
- W.M. Sanderson, F. Wang, J. Schrier, W.E. Buhro, and R.A. Loomis*, “Intraband Relaxation Dynamics of Charge Carriers within CdTe Quantum Wires”, *J. Phys. Chem. Lett.*, **11**, 4901-10 (2020).
- W.M. Sanderson, J. Hoy, C. Morrison, F. Wang, Y. Wang, P.J. Morrison, W.E. Buhro, and R.A. Loomis*, “Excitation Energy Dependence of Photoluminescence Quantum Yields in Semiconductor Nanomaterials with Varying Dimensionalities”, *J. Phys. Chem. Lett.*, **11**, 3249-56 (2020).
- N. Zeigler, C. Makarem, J. Wei, and R.A. Loomis*, “Electronic Predissociation in Rare Gas-Dihalogen Complexes”, *J. Chem. Phys.*, **152**, 094303 (2020).

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ASSOCIATE PROFESSOR
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Physical Chemistry

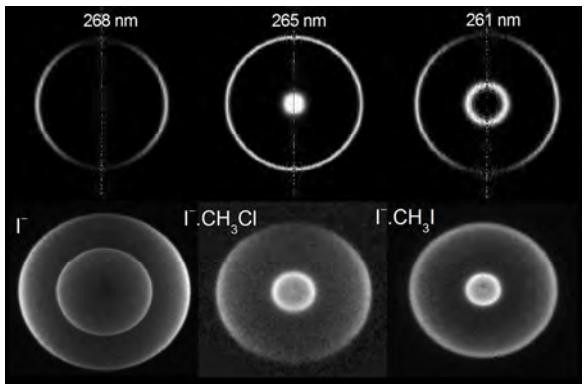
Richard Mabbs

Postdoctoral Research Associate, University of Arizona (2002-5); Ph.D., University of Nottingham (1995); B.Sc. University of Nottingham (1990).

Our research interests focus on electron-molecule, electron-atom, and ion-molecule interactions, the dynamics of reactions induced by electron capture and photoexcitation, and the electronic structure of atoms, molecules, and ions. We use an anion photodetachment approach and velocity mapped photo-

electron imaging complimenting our experimental studies with quantum chemistry calculations. To learn more about our research, instrumentation and group members please visit <http://www.chemistry.wustl.edu/~mabbs/>

Typically we prepare anionic species and electrons are removed via laser excitation, leaving the neutral species behind. A 2D projection (image) of the initial 3D distribution in momentum space is obtained using a position sensitive detector. The original 3D photoelectron velocity distribution can be mathematically extracted. We retrieve the photoelectron spectrum (which allows determination of the electronic eigenvalues of the system) and the angular distribution of the electrons. The spatial distribution is particularly interesting as it allows us to infer the nature of the parent electronic wavefunction at the instant of detachment. Hence an image represents a signature of the parent orbital. The example shown to the right compares detachment from Br^- (electron removed from a 4p orbital) with detachment from Cu^- (electron removed from the 4s orbital). The distribution of the electrons with respect to the polarization axis (ϵ_p) of the laser is markedly different in each case.



Top row, the $\text{I}^-(\text{CH}_3)_2\text{CO}$ detachment angular distribution undergoes a dramatic change between photon wavelengths 268 and 261 nm due to the presence of a dipole supported, temporary state of the cluster framework. Bottom row, 280 nm detachment from I^- and $\text{I}^-\text{CH}_3\text{Cl}$ displays remarkably similar angular distributions (outer feature in images). However, the $\text{I}^-\text{CH}_3\text{I}$ photoelectron angular distribution at this wavelength is nearly isotropic, the result of a σ^* resonance associated with the CH_3I molecule.

Bottom row, the $\text{I}^-(\text{CH}_3)_2\text{CO}$ detachment angular distribution undergoes a dramatic change between photon wavelengths 268 and 261 nm due to the presence of a dipole supported, temporary state of the cluster framework. Bottom row, 280 nm detachment from I^- and $\text{I}^-\text{CH}_3\text{Cl}$ displays remarkably similar angular distributions (outer feature in images). However, the $\text{I}^-\text{CH}_3\text{I}$ photoelectron angular distribution at this wavelength is nearly isotropic, the result of a σ^* resonance associated with the CH_3I molecule.

Knowledge of free anion photoelectron angular distributions allows us to obtain insight into the interaction of free electrons with neutral molecules. Photoexcitation within a physically bound cluster, typically comprising an atomic anion and a target molecule, effectively fires the excess electron at the target. In the absence of a target molecule the photoelectron angular distribution is determined by the originating (s, p, d) orbital. However, if there is significant interaction with the target molecule the angular distribution is significantly altered. Such studies are particularly sensitive to the electron-molecule resonances which lead to strong scattering of electrons and play a vital role in electron capture induced chemistry. These resonances are often highly energy dependent and the angular distribution often undergoes a rapid change with a narrow range of electron kinetic energies.

Time Resolved Studies. Using photodetachment imaging in conjunction with an ultrafast laser pump-probe scheme we can follow reactions on the timescale of atomic motion. The first, or pump photon initiates dissociation by excitation of an anionic species to a dissociative electronic state. The second (probe) laser pulse (delayed by 10's - 100's of fs with respect to the pump) is used to photodetach the excess electron. In particular, the changing photoelectron angular distributions track the evolution of the electronic wavefunctions from those of reactants into those of products. Furthermore, application of a pump-probe scheme to cluster anion excitation affords the opportunity to study electron collision induced dissociative processes on the timescale of molecular motion. These low energy electron transfer induced processes are of widespread importance, including plasma pollutant processing technologies, ionospheric chemistry and biological tissue damage due to ionizing radiation.

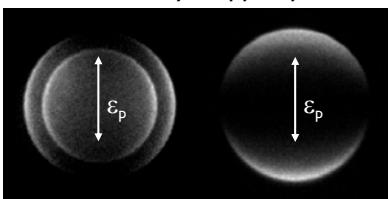
Selected Publications

- C.A. Hart and R. Mabbs*, "Stabilized Resonance are No Less Exciting." *Nature Chemistry*, **13**, 721-2 (2021).
- J. Lyle, T.C. Jagau, R. Mabbs*, "Spectroscopy of Temporary Anion States: Renner-Teller Coupling and Electronic Autodetachment in Copper Difluoride Anion." *Faraday Discussions*, **217**, 533-46 (2019).
- J. Lyle, S.R. Chandramoulee, J.R. Hamilton, B.A. Traylor, T.L. Guasco, T.C. Jagau, R. Mabbs*, "Characterization of the Vibrational Properties of Copper Difluoride Anion and Neutral Ground States via Direct and Indirect Photodetachment Spectroscopy." *J. Chem. Phys.*, **149**, 084302 (2018).
- J. Lyle, S.R. Schandramoulee, C.A. Hart, and R. Mabbs, "Photoelectron Imaging of Anions Illustrated by 310 nm Detachment of F^- ." *Jove - Journal of Visualized Experiments*, **137**, e57989 (2018).
- J. Lyle, O. Wedig, S. Gulania, A.I. Krylov, R. Mabbs*, "Channel Branching Ratios in CH_2CN^- Photodetachment: Rotational Structure and Vibrational Energy Redistribution in Autodetachment." *J. Chem. Phys.*, **147**, 234309 (2017).

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Br^- (left) and Cu^- (right) photoelectron images. The distributions reflect 4p (Br^-) or 4s (Cu^-) orbital detachment.



PROFESSOR

Organic Chemistry, Synthetic Chemistry

Kevin D. Moeller

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NIH Postdoctoral Fellow, University of Wisconsin - Madison (1985); Ph.D., University of California Santa Barbara (1985); B.A., University of California, Santa Barbara (1980).

ACS Arthur C. Cope Scholar Late Stage Career Award (2020); ACS Midwest Award (2019); Manuel M. Baizer Award for Contributions to Organic Electrochemistry: Division of Organic and Biological Electrochemistry, the Electrochemical Society (2016); ACS St. Louis Award (1997); Wash. U. Student Union - A&S Professor of the Year (2001).

What are the “tools” that allow us to construct molecules, and are these “tools” capable of building what we need in a timely and efficient manner? These two questions provide the motivation for our group’s exploration of electrochemistry, an exploration that has led us to pursue two broad areas of research:

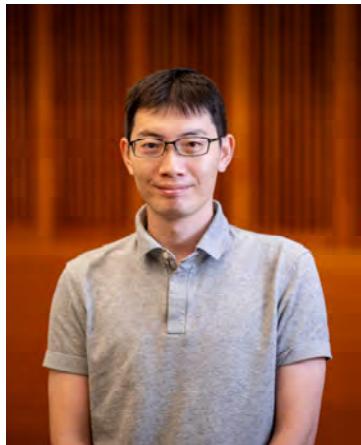
New Synthetic Methodology/Organic Synthesis: Because electrochemistry enables the selective manipulation of molecular oxidation states, the generation of highly reactive intermediates, and the reversal of functional group polarity, it provides an ideal method for discovering and exploring new, synthetically useful reaction. For instance, consider this generalized reaction: a electron-rich, normally nucleophilic enolate equivalent is oxidized leading to the formation of an electrophilic radical cation. The radical cation traps a second nucleophile leading to the formation of a new bond and ring. To date, a number of such reactions have been developed as synthetic tools. Several recent examples are illustrated in Scheme I. The electrochemical reactions do not require the use of highly specialized equipment. All of the reactions shown can be performed in a three neck round bottom flask using a 6V lantern battery as a power supply and a total reaction set up (minus the flask) costing less than \$6.

New Analytical Tools for Probing Molecular Interactions: While the chemistry outlined above has proven very useful for solving a number of structural challenges in synthesis, not all synthetic challenges in organic chemistry are of a “structural variety”. Instead some are of a logistical nature. For example, as part of a long standing effort to “map” the preferred three-dimensional binding motifs of biological receptors, we recently became engaged in an effort to develop methods for monitoring ligand-receptor binding events in real time. To accomplish this goal, potential ligands (small molecules, peptidomimetics, glycoproteins, etc.) will be placed or synthesized on microelectrode arrays so that each unique molecular ligand is located proximal to a unique, individually addressable electrode in the array. The electrodes in the array will then be used to monitor binding events between the potential ligands and various biological receptors.

Work on this project is continuing along several paths. New site-selective synthetic methods are being explored, site-selectively cleavable linkers are being developed for characterizing molecules on the surface of an array, strategies for determining in “real-time” the relative binding of molecular ligands to various biological receptors are being studied, new custom polymers for coating the arrays and controlling the surface used for the subsequent synthetic and analytical experiments are being synthesized, and studies aimed at expanding the utility of the microelectrode arrays as bioanalytical tools are being pursued.

Selected Publications

- T. Wu and K.D. Moeller*, “Organic Electrochemistry: Expanding the Scope of Paired Reactions.” *Angewandte Chemie Int. Ed.*, **60**, 12883-90 (2021).
- M.D. Graaf, L. Gonzalez, Z. Medcalf, and K.D. Moeller*, “Using a Combination of Electrochemical and Photoelectron Transfer Reactions to Gain New Insights into Oxidative Cyclization Reactions.” *J. Electrochemical Society*, **167**, 155520 (2020).
- R. Francke, L. Gonzalez, R.D. Little, K.D. Moeller*, “Electrons, Electrodes, and the Transformation of Organic Molecules.” *Surface and Interface Science: Volume 10: Applications of Surface Science II, Volume 10, Chapter 79*, (2020).
- Q. Jing and K.D. Moeller*, “From Molecules to Molecular Surfaces. Exploiting the Interplay Between Organic Synthesis and Electrochemistry.” *Acc. Chem. Res.* **53**, 135-43 (2020).
- N.-H. Yeh, Y. Zhu, and K.D. Moeller*, “Electroorganic Synthesis and the Construction of Addressable Molecular Surfaces.” *ChemElectroChem*, **6**, 4134-43 (2019).



ASSISTANT PROFESSOR

Biophysical Chemistry , Solution-state NMR, Protein-ligand/protein-protein interactions
Protein hydration, Neurodegenerative diseases

Yusuke Okuno

PHD, University of Wisconsin at Madison
BS, University of Illinois at Urbana-Champaign

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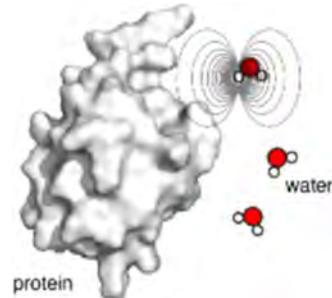
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The Okuno research group aims to develop both the theoretical and experimental methods needed to understand the chemicophysical nature of ligand-protein and protein-protein interactions at the molecular level.

We put emphasis on understanding the roles of solvent (e.g., water) and weak noncovalent interactions such as NH- π and CH- π interactions in ligand-protein and protein-protein binding processes. Nuclear Magnetic Resonance Spectroscopy (NMR) is a powerful technique that provides atomic-level information about proteins and protein interactions. We use NMR spectroscopy as well as other experimental and computational approaches to unravel challenging biological processes.

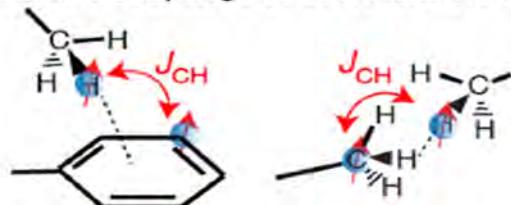
Current projects in the lab include:

The role of water in protein-ligand association Water is the most abundant molecule in any biological system. Elucidating the molecular details of how water molecules interact with proteins is therefore critical for understanding any types of biological processes. By taking advantage of the fact that water molecules generate weak magnetic fields, we investigate how water molecules interact with a protein at the atomic level. For example, NMR observable known as the nuclear Overhauser effect (NOE) provides rich information about both the dynamic and energetic of water-protein interactions. We aim to develop new experimental methods to detect weak water-NOE signals and develop a theoretical basis to rigorously interpret the experiments.



The weak noncovalent protein-ligand interactions in IDP Many drugs and other small molecule ligands utilize weak noncovalent interactions to bind to their targets. For example, many drugs consist of aromatic groups capable of NH- π and/or CH- π interactions with a protein surface.

Scalar J couplings of CH- π and CH/CH



NMR spectroscopy enables direct detections of NH- π , CH- π , and CH-CH interactions at atomic resolution by so-called "through-space" J -coupling. The J -coupling can be detected only when there is an electron cloud between the two nuclei, thereby providing the direct evidence of the existence of hydrogen bonds. We aim to develop new experimental methods to measure through-space J -coupling tailored to probe ligand-protein interactions.

Probing the molecular forces in protein aggregation and in liquid-liquid phase separation The amyloid beta peptides known as A β (1-42) and A β (1-40) rapidly form aggregation species and the aggregates are known to be involved in Alzheimer's disease. Many drugs are targeted to prevent these aggregation pathways of A β peptides. However, not much is known about the mechanisms of how A β peptides form these aggregates at the molecular level. Using the NMR as well as other experimental techniques, we explore what chemical forces drive the early stage of A β peptides aggregation processes with the ultimate goal to develop a new therapy for Alzheimer's diseases and other neurodegenerative diseases.

Selected Publications

- Okuno, Y., Schwieters, C.D., Yang, Z., Clore, G.M. Theory and Applications of Nitroxide-based Paramagnetic Cosolutes for Probing Intermolecular and Electrostatic Interactions on Protein Surfaces. *J. Am. Chem. Soc.*, 144 (46), 21371-21388
- Okuno, Y., Yoo, J., Schwieters, C.D., Best, R.B., Chung, H.S. & Clore, G.M. Atomic view of cosolute-induced protein denaturation probed by NMR solvent paramagnetic relaxation enhancement. *Proc. Natl. Acad. Sci.* 118, e2112021118
- Okuno, Y., Szabo, A., Clore, G. M. Quantitative interpretation of solvent paramagnetic relaxation for probing protein–cosolute interactions. *J. Am. Chem. Soc.* 2020, 142 (18) 8181-8290
- Okuno, Y., Mecha, M. F., Cavagnero, S. Laser-and cryogenic probe-assisted NMR enables hypersensitive analysis of biomolecules at submicromolar



**PROFESSOR, MICHAEL AND TANA POWELL
PROFESSOR OF CHEMISTRY**

Biological and Physical Chemistry, Medicine,
Genetics

Gary J. Patti

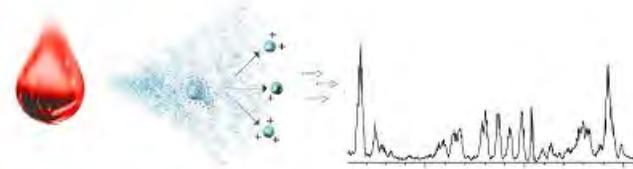
NIH Postdoctoral Fellow, The Scripps Research Institute (2008-11); Ph.D., Washington University (2008); B.A., St. Louis University (2002).

NIH Clinical Research LRP Award, National Institute on Aging (2010); Society for Neuroscience Presentation Award, San Diego Chapter (2010); American Aging Association Research Award (2010); American Library Association Innovation Award Finalist (2009); NMR Graduate Research Award, Isotec (2007).

Our laboratory is interested in the biochemical reactions that underlie fundamental physiological processes and associated metabolic derangements that cause disease. By using state-of-the-art mass spectrometers coupled with cutting-edge metabolomic technologies, we take a systems-level approach to study comprehensive metabolism and identify specific pathways that are altered in connection with particular phenotypes. We strive to translate our metabolomic findings into a physiological context through the use of classical biochemical tools and animal models as well as with the development of new technologies such as mass spectrometry-based metabolite imaging and whole-cell NMR. Our specific interests are outlined below.

Metabolomics: Advancing Technology for Biological Discovery:

Modern day mass spectrometers enable the detection of thousands of compounds in the metabolic extract of biological samples with unprecedented sensitivity. The goal of metabolomics is to compare these data across different sample types to gain insight into the metabolic programs that govern distinct biological phenotypes. A major challenge in the field, however, has been the translation of mass spectrometric peaks into metabolic structures and pathways. Indeed, the masses of more than half of the peaks routinely detected from biological samples in our laboratory return no hits when searched in currently available metabolomic databases. A major effort of our research program is to develop new metabolomic technologies that improve the throughput of structural identifications as well as our ability to characterize the pathway, physiological function, and anatomical localization of metabolites that do not fit into canonical metabolic reaction maps. To accomplish these goals, we rely heavily on bioinformatic strategies and modified LC/MS/MS experimental methodologies. Additionally, our strategies include mass spectrometry-based metabolite imaging, whole-cell NMR, and integration with sequencing data.



Cancer: It is well established that most cancer cells take up an increased amount of glucose relative to that taken up by normal differentiated cells. This phenomenon, known as the Warburg effect, is also observed in other rapidly dividing cells. It is speculated that Warburg metabolism in proliferating cells supports the metabolic demands of cellular growth. However, the fates of glucose and other nutrients taken up by cancer cells have not been comprehensively mapped. We are interested in using untargeted metabolomic technologies to quantitatively determine how cancer cells metabolize nutrients differently than normal differentiated cells. In addition to examining the well-studied pathways of central carbon metabolism, we also seek to study peripheral metabolic pathways and pathways involving unknown compounds that have yet to be characterized.

Environmental Health: There are tens of thousands of chemicals in widespread commercial use. The effects of most of these compounds on health are unknown. Although high-throughput assays have emerged to screen chemicals for potentially hazardous effects, these platforms do not have molecular-level resolution and therefore cannot reveal mechanisms of toxicant action. However, determining toxicant mechanisms of action is highly valuable as this information can help predict if other chemicals are hazardous, provide insight into therapies to treat toxicant exposure, or facilitate the development of safer man-made chemicals. Untargeted metabolomics is ideally suited to reveal toxicant mechanisms of action. By measuring the levels of thousands of metabolites, it can reveal specific enzymes and pathways that are disrupted upon toxicant exposure.

Chronic Pain: Our laboratory is interested in neuropathic pain, a chronic pain state that results from peripheral and/or central nerve injury. By using untargeted metabolomics, we have identified a novel sphingolipid, N,N-dimethylsphingosine (DMS), that is increased in the dorsal horn of rats suffering from neuropathic pain and is sufficient in itself to induce pain-like behaviors when administered intrathecally in healthy rats. A major effort in our laboratory is to identify the metabolic pathways and specific enzymes involved in DMS biosynthesis as well as the biochemical mechanism(s) by which DMS elicits pain-like behavior. Based on preliminary data showing that DMS results in cytokine release from astrocytes in vitro, we are interested in dissecting the role of astrocytes in the neuropathic pain state and the metabolic interrelationships with other surrounding cell types that may be influenced by alterations in sphingolipid production.

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Organic Chemistry, Computational Chemistry Jay W. Ponder



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NIH Postdoctoral Fellow, Yale University (1985-90); Ph.D., Harvard University (1984); B.S., Wabash College (1978).

Chairman-Elect, Computational Chemistry Gordon Research Conference (2012); Scientific Advisory Board, Numerate, Inc., Algodign, LLC (2007).

Research in my group focuses on computational chemistry. We are involved in application of software tools addressing problems in structural biology, protein engineering, organic chemistry and materials science. The lab has developed several software suites ranging from macromolecular mechanics and dynamics simulation (TINKER), to empirical packing analysis of protein structure (PROPAK), to sequence level analysis and characterization (SLEUTH), to *ab initio* protein structure prediction (DISTGEOM). Much recent effort has focused on parameterization, validation and application of a new polarizable atomic multipole molecular mechanics force field. We also collaborate on parallelization of algorithms and software for molecular simulation.

Improved Molecular Mechanics Force Fields. We have implemented efficient methods for including multipole electrostatics and polarization in simulations as the framework for our next-generation AMOEBA (*Atomic Multipole Optimized Energetics for Biomolecular Applications*) force field. AMOEBA enables reliable calculation of structures and has significant advantages over traditional fixed partial atomic charge models such as Amber and CHARMM. The next improvements to the AMOEBA model will include accounting for charge transfer and penetration effects. Accurate potential functions for these important electrostatic effects are being developed and parameterized.

Host-Guest and Protein-Ligand Binding Energies. A “grand challenge” for computational chemistry is calculation of binding free energies to within “chemical accuracy”- absolute errors of 0.5 kcal/mol or less. Reliable computational results would be of tremendous utility in computer-aided drug design, materials engineering, and many other fields. We are investigating the cucurbituril family of “host” molecules, and modeling their affinity for a variety of organic “guests”. The cucurbiturils are excellent model systems since they are relatively small and rigid, and contain the amide and aromatic moieties involved in protein structure and biomolecular recognition.

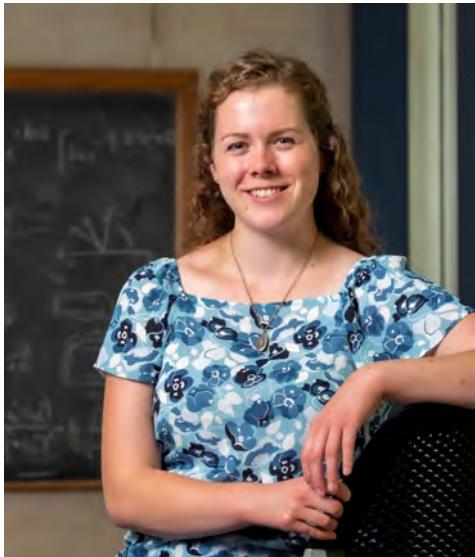
Crystal Structure Prediction. Due to the limited search space, small molecule crystal prediction is easier than the classical “protein folding problem”. Indeed, great progress has been made over the past five years; some of it using advanced force field methodology similar to AMOEBA. Our “reductionist” approach to understanding protein structure and folding is to first model peptide crystals, which exhibit many of the same structural features found in typical globular proteins.

Protein Modeling and Engineering. Current biomolecular applications include elucidation of the role of ions in biology, and refinement of homology models. We are presently testing new valence bond and angular overlap approaches to transition metal ligand field effects within a molecular mechanics framework, with the goal of modeling metalloprotein structure and function. Ultimately, a major interest for our group lies in the “end game” of protein folding- making a connection between atomic-level protein structures and low-resolution models from homology or fold recognition algorithms.

Novel Methods for Conformational Search. We are exploring powerful approaches to conformational search for flexible biopolymers. One method transforms potential energy surfaces by a diffusion equation-based potential smoothing procedure. This paradigm is applicable to many problems: transmembrane helix packing, global optimization, and energy-based conformational clustering. Another method uses a novel distance geometry algorithm and heuristics to predict protein structure. Statistical distance distributions and secondary structure constraints generate libraries of candidate folds to be scored with an informatics-based contact function or physics-based potential of mean force.

Selected Publications

- J.Y. Xiang and J.W. Ponder, A Valence Bond Model for Aqueous Cu and Zn Ions in the AMOEBA Polarizable Force Field, *J. Comput. Chem.*, **33**, (2012).
- P. Ren, C. Wu and J. W. Ponder, Polarizable Atomic Multipole-based Molecular Mechanics for Organic Molecules, *J. Chem. Theory Comput.*, **7**, (2011) .
- H. L. Woodcock, B. T. Miller, M. Hodoscek, A. Okur, J. D. Larkin, J. W. Ponder and B. R. Brooks, MSCALE: A General Utility for Multiscale Modeling, *J. Chem. Theory Comput.*, **7**, 1208-1219 (2011).
- Y. Shi, C. Wu, J. W. Ponder and P. Ren, Multipole Electrostatics in Hydration Free Energy Calculations, *J. Comput. Chem.*, **32**, 967-977 (2011).
- J. W. Ponder, C. Wu, P. Ren, V. S. Pande, J. D. Chodera, D. L. Mobley, M. J. Schnieders, I. Haque, D. S. Lambrecht, R. A. DiStasio, Jr., M. Head-Gordon, G. N. I. Clark, M. E. Johnson and T. Head-Gordon, Current Status of the AMOEBA Polarizable Force Field, *J. Phys. Chem. B*, **114**, 2549-2564 (2010).
- N. A. Baker, P. Ren and J. W. Ponder, Polarizable Atomic Multipole Solutes in a Poisson-Boltzmann Continuum, M. J. Schnieders, *J. Chem. Phys.*, **126**, 124114 (2007).
- T. D. Rasmussen, P. Ren, J. W. Ponder and F. Jensen, Force Field Modeling of Conformational Energies: Importance of Multipole Moments and Intramolecular



ASSISTANT PROFESSOR

Inorganic materials synthesis, Metastable materials, Nanomaterials, Quantum materials, Magnetism and non-trivial topology

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Kelly Powderly

Beckman-Brown Interdisciplinary Postdoctoral Fellow, University of Illinois Urbana-Champaign

PHD, Chemistry and Materials Science, Princeton University

BA, Chemistry and Integrated Science, Northwestern University

Awards & Honors

2023 Beckman-Brown Interdisciplinary Postdoctoral Fellowship, 2022 Solid State Chemistry Gordon Research Seminar Invited Speaker, 2020 Princeton University Pickering Teaching Award, 2017 NSF Graduate Research Fellowship

The Powderly Group seeks to develop and utilize new synthetic pathways to discover extended solids with magnetic, electronic, and non-trivial topological properties of interest in quantum information science and to explore new fundamental bonding in materials.

Conventional syntheses of solid-state materials require high temperatures ($>800\text{ }^{\circ}\text{C}$) and long heating times (days to weeks) to allow atoms to diffuse and form the most thermodynamically stable phase(s) at that temperature. Many interesting materials have been discovered under these conditions; however, certain combinations of atomic structures and elemental compositions, which may give rise to desirable electronic and magnetic properties, are not accessible with conventional solid-state synthesis. We will employ alternative synthetic methods, including solution-phase synthesis to facilitate diffusion, high pressure to shift the thermodynamic landscape, and assembly of pre-synthesized building blocks for “designer” structures, to access metastable materials that exhibit quantum spin liquid behavior, superconductivity, and non-trivial topology.

Our research focuses on:

1. developing synthetic protocols and probing reactions *in situ* to discover new metastable materials, which form under non-traditional synthetic conditions and may be “trapped” at ambient pressure and room temperature;
2. solving their crystal structures and investigating their magnetic, electronic, and thermal responses to explore properties of interest in quantum information science;
3. collaborating with physicists and engineers to further study our materials under extreme conditions and in new devices.

Specific research directions include:

- Design and assembly of 2D spin-nets from molecular cluster precursors
- *In situ* study of diffusion-suppressed routes to intermetallics
- High-pressure metathesis for new noble-gas solids

In the Powderly group, researchers will learn and apply synthetic and characterization techniques including solution-phase synthesis of nanoclusters and metal complexes, *in situ* X-ray diffraction and thermal analysis to probe solid-state transformations up to $1000\text{ }^{\circ}\text{C}$, high-pressure solid-state ion-exchange reactions in diamond anvil cells, and variable-temperature magnetic, electronic, and thermal characterization to explore materials’ quantum behaviors.

Selected Publications

Powderly, K. M.; Zhang, Q.; Devlin, K. P.; Gui, X.; Ni, D.; Xie, W.; Cava, R. J. [Quasi-one-dimensional \$\text{Pb}_5\text{Re}_3\text{O}_{15}\$: A 5d realization of the Heisenberg antiferromagnetic spin-1/2 chain.](#) *Phys. Rev. Mater.* **2023**, *7*, 114408.

Greskovich, K. M.;* **Powderly, K. M.**;* Kincanon, M. M.; Forney, N. B.; Jalomo, C. A.; Wo, A.; Murphy, C. J. [The Landscape of Gold Nanocrystal Surface Chemistry](#). *Acc. Chem. Res.* **2023**, *56*, 1553 – 1564.



ASSISTANT PROFESSOR

Biological and Physical Chemistry

Courtney Reichhardt

Postdoctoral Fellow, Department of Microbiology at the University of Washington (2016-2021); Ph.D., Stanford University (2016); B.S., Montana State University (2010).

K99/R00 "Pathway to Independence" Award, NIGMS (2019); Postdoc-to-Faculty Transition Award, Cystic Fibrosis Foundation (2019); Cystic Fibrosis Mentored Research Innovation Award (2019); Carol Basbaum Memorial Research Fellowship (2017).

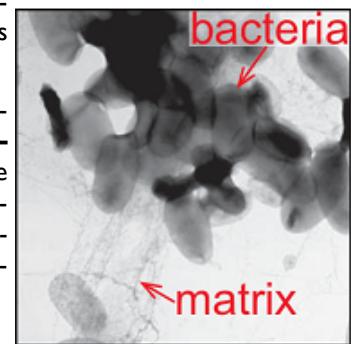


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The overarching goal of the Reichhardt Lab is to **discover the fundamental biophysical principles of biofilm assembly**. Within biofilms, aggregates of microbes are encased in a mesh-like, biopolymer-rich matrix that promotes microbial cell-cell interactions, adherence to host tissues, and protection from antimicrobials. These properties contribute to biofilms causing difficult-to-treat chronic infections.

Despite the importance of the biofilm matrix, we still do not understand how individual matrix components are assembled into a functional architecture. **Since this problem spans several scales—multicellular to atomic—new multidisciplinary approaches are required.** Therefore, we are developing approaches that integrate microbiological methods with physical chemistry tools including microscopy and solid-state nuclear magnetic resonance (NMR). Overall, our research program aims to provide critical understanding of biofilm assembly, with broader impact on bacterial physiology, materials science, and treatment for chronic infections.

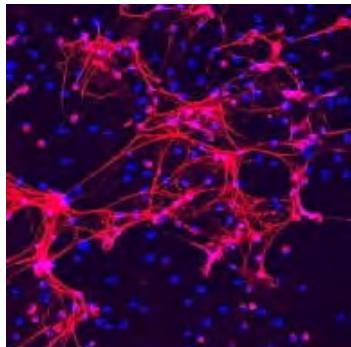
Biofilm Matrix Dynamics. Biological materials—including the biofilm matrix—are dynamic, with properties and functions that change in response to environmental cues. We are applying solid-state NMR and microscopy to explore how biofilm matrix interactions change over the course of the biofilm lifecycle.



Transmission electron micrograph of a biofilm.

Biofilms in CF Lung Infections. People with cystic fibrosis (CF) have recurrent lung infections that are thought to be biofilm-involved infections. We are using innovative interdisciplinary approaches to provide critical understanding of biofilm assembly in CF lung infections.

Integration of Host Material into Biofilms: An incredibly important feature of biofilm infections is the host environment. However, in general, only self-produced biofilm matrix has been characterized. We are developing solid-state NMR and microscopy approaches to examine total infection-relevant biofilm composition.



Neutrophil extracellular traps (NETs). Photo credit: NIAMS Systemic Autoimmunity Branch, Maria J. Kaplan

Selected Publications

- L.K. Jennings, J.E. Dreifus, C. Reichhardt, K.M. Storek, P.R. Secor, D.J. Wozniak, K.B. Hisert, M.R. Parsek*, "Pseudomonas Aeruginosa Aggregates in Cystic Fibrosis Sputum Produce Exopolysaccharides That Likely Impede Current Therapies." *Cell Reports*, **34**, 108782 (2021).
- E. Limqueco, D. Passos Da Silva, C. Reichhardt, F. Su, D. Das, J. Chen, S. Srinivasan, A. Convertine, S.J. Skerrett, M.R. Parsek*, P.S. Stayton*, and D.M. Ratner*, "Mannose Conjugated Polymer Targeting P. Aeruginosa Biofilms." *ACS Infectious Diseases*, **6**, 2866-2871 (2020).
- C. Reichhardt, H.M. Jacobs, M. Matwichek, C. Wong, D.J. Wozniak, and M.R. Parsek*, "The Versatile Pseudomonas Aeruginosa Biofilm Matrix Protein CdrA Promotes Aggregation Through Different Extracellular EPS Interactions." *Journal of Bacteriology*, **202**, e00216-20 (2020).
- C. Reichhardt and M.R. Parsek*, "Confocal Laser Scanning Microscopy for Analysis of Pseudomonas Aeruginosa Biofilm Architecture and Matrix Localization." *Frontiers Microbiology*, **10**, 677 (2019).
- D. Passos da Silva, M.L. Matwichek, D.O. Townsend, C. Reichhardt, D. Lamba, D.J. Wozniak, and M.R. Parsek*, "The Pseudomonas Aeruginosa Lectin LecB Binds to Psl and Stabilizes the Biofilm Matrix." *Nature Communications*, **10**, 2183 (2019).
- C. Reichhardt, C. Wong, D. Passos da Silva, D.J. Wozniak, and M.R. Parsek*, "CdrA Interactions within the Pseudomonas Aeruginosa Biofilm Matrix Safeguard It From Proteolysis and Promote Cellular Packing." *mBio*, **9**, e01376-18 (2018).
- B.S. Tseng, C. Reichhardt, G.E. Merrihew, J.J. Harrison, M.J. MacCoss, and M.R. Parsek*, "A Biofilm Matrix-associated Protease Inhibitor Protects Pseudomonas Aeruginosa from Proteolytic Attack." *mBio*, **9**, e00543-18 (2018).
- C. Reichhardt* and L. Cegelski*, "The Congo Red Derivative FSB Binds to Curli Amyloid Fibers and Specifically Stains Curliated." *E. coli. PLOS ONE*, **13**, e0203226 (2018).
- C. Reichhardt, D.A. Stevens, and L. Cegelski*, "Fungal Biofilm Composition and Opportunities in Drug Discovery." *Future Medicinal Chemistry*, **8**, 1455-1468 (2016).



PROFESSOR OF CHEMISTRY AND PHYSICS

Nuclear Chemistry

Lee G. Sobotka



Postdoctoral Research Associate, University of California, Berkeley and Lawrence Berkeley Laboratory (1982-4); Ph.D., University of California, Berkeley (1982); B.S., University of Michigan (1977).

Fellow of the American Physical Society, Division of Nuclear Physics (2010); ACS Seaborg Award in Nuclear Chemistry (2010); NSF Presidential Young Investigator Award (1986).

Professor Sobotka is particularly interested in the de-excitation modes of highly-excited nuclei; continuum structure of exotic nuclei; nucleosynthesis, dynamics of nuclear fusion and fission; the asymmetry dependence nucleon correlations in atomic nuclei; the asymmetry dependence of the equation of state of nuclear matter; multi-particle correlations; advanced radiation detectors and the associated electronics including ASIC design; and various applied nuclear science topics.

Our interests span from basic nuclear science to selected topics in applied nuclear science. Topics under current investigation include:

- The continuum structure of light nuclei both on and off nucleosynthetic paths.
- The influence of phase transitions in finite, two-component quantal systems on the dynamics of collisions between heavy nuclei.
- Developing techniques to measure the evolution of the nuclear density-of-states with excitation energy.
- Clustering in low-density nuclear systems.
- The deexcitation of highly-excited nuclei by the emission of complex clusters of nucleons.
- Development of new detector technologies and pulse-processing electronics for ionizing radiation.
- Employing multiple techniques (including ^{11}C positron imaging) to study how the products of photorespiration are used by plants to direct plant physiology.

Related to the second topic, nuclear systems are two component (n and p) quantal systems. When taken through a phase transition, quantal systems must obey the same Gibbs' conditions (equality of the chemical potentials of each substance in the phases in equilibrium) as non-quantal systems. The common component fractionation (distillation) with phase separation can also occur in multicomponent quantal systems. It is just such a component fractionation (different n/p ratios in the low and high-density regions of a reaction system), driven solely by quantal effects, that has drawn our interest. The thermodynamic force driving such a fractionation can be understood as follows. Imagine an unequal filling of dual sets of quantum levels, one set for n's the other for p's. As a result of the different Fermi levels, there is a finite thermodynamic potential difference between n's and p's. Given enough time the Weak interaction will convert n's to p's (or visa-versa) to equalize the Fermi energies. This is in fact what drives b-decay. However due to the weakness of the interaction, such interconversions have characteristic times exceeding 1 ms.

On a shorter time scale, fractionation should occur if two "phases" of different density are present. The phase with lower density will have the quantum levels spaced closer together and thus a particle imbalance will result in a smaller absolute chemical potential difference. If the two phases of different density are in equilibrium, the nucleon species in excess will be driven into the low-density phase (where the absolute difference in the Fermi levels is smaller.) Both theoretical modeling and experiments related to generating conditions under which such a fractionation could occur are topics of current interest.

Needless to say, this topic is closely related to the Equation of State (EoS) of asymmetric nuclear matter. Decoding this EoS is essential for determining the structure of neutron stars and the nature of super-nova explosions. These stellar explosions are the likely mechanisms for the synthesis of about half of the heavy elements via the rapid-neutron-capture process. In this process, the explosion generates an intense pulse of neutrons which are sequentially captured by seed nuclei. After the neutron pulse subsides, the very neutron-rich species b-decay back to stability. This element building process is controlled by the masses and the density of states (at the energy corresponding to the capture of a neutron) of the b-unstable, neutron-rich nuclei.

Selected Publications

- R. J. Charity, et al., "Using Spin Alignment of Inelastically Excited Nuclei in Fast Beams to Assign Spins: The Spectroscopy of ^{13}O as a Test Case." *Phys. Rev. C*, **104**, 024325 (2021).
- J. Manfredi, et al., "Quenching of Single-particle Strengths in Direct Reactions." *Phys. Rev. C*, **104**, 024608 (2021).
- J. Bishop, et al., "Evidence Against the Efimov Effect in ^{12}C from Spectroscopy and Astrophysics." *Phys. Rev. C*, **103**, L051303 (2021).
- R.J. Charity, et al. "Observation of the Exotic Isotope ^{13}F Located Four Neutrons Beyond the Proton Drip Line." *Phys. Rev. Lett.*, **126**, 132501 (2021)



PROFESSOR

Bioorganic Chemistry

John-Stephen A. Taylor

Postdoctoral Research Associate, California Institute of Technology (1981-3); Ph.D., Columbia University (1981); B.S., Massachusetts Institute of Technology (1976).



Professor Taylor's current research interests include bioorganic and nucleic acids chemistry, breast cancer imaging and chemotherapy, sunlight and skin cancer, and natural products inhibiting or activating heat shock proteins.

Professor Taylor's research on sunlight and skin cancer has shown that although many of the carcinogenic effects of sunlight can be attributed to DNA photoproducts, such as the cis-syn cyclobutane pyrimidine dimer (CPD), the factors governing the formation and biological activities of individual photoproducts are largely unknown. We are currently most interested in understanding a newly discovered "dark" or chemosensitization pathway (Fig. 1) to CPDs in melanocytes involving high energy dioxetanes. We are also studying what controls deamination of cis-syn cyclobutane pyrimidine dimers at CpG sites in nucleosome core particles as a model of chromatin (Fig. 2). We have also recently discovered a new photoproduct of human telomeric DNA which arises from G-quadruplex structures in vitro (Fig. 3) and have been investigating the possible roles of the photoproduct in vivo. This work involves computational chemistry, organic synthesis, synthesis of fluorescent probes, automated DNA synthesis, HPLC, 2D NMR, MALDI and ESI, radioactive labeling, gel electrophoresis, NextGen sequencing, cloning, protein expression, cell culture, and PCR.

Selected Publications

- C. Lu, N.E. Gutierrez-Bayona, J.-S. Taylor*, "The Effect of Flanking Bases on Direct and Triplet Sensitized Cyclobutane Pyrimidine Dimer Formation in DNA Depends on the Dipyrimidine, Wavelength and the Photosensitizer", *Nucleic Acids Researc*, **49**, 4266-80 (2021).
- J.E. Smith-Carpenter and J.-S. Taylor*, "Photocrosslinking of G-Quadruplex-Forming Sequences found in Human Promoters", *Photochemistry and Photobiology*, **85**, 252-66 (2019).
- C. Lu, J.E. Smith-Carpenter, and J.-S. Taylor*, "Evidence for Reverse Hoogsteen Hairpin Intermediates in the Photocrosslinking of Human Telomeric DNA Sequences", *Photochemistry and Photobiology*, **94**, 685-97 (2018).
- K. Wang and J.-S. Taylor*, "Modulation of Cyclobutane Thymine Photodimer Formation in T11-tracts in Rotationally Phased Nucleosome Core Particles and DNA Minicircles", *Nucleic Acids Research*, **45**, 7031-41 (2017).
- J.-S. Taylor*, "Design, synthesis, and characterization of nucleosomes containing site-specific DNA damage", *DNA Repair*, **36**, 59-67 (2015).
- V.J. Cannistraro, S. Pondugula, Q. Song, and J.-S. Taylor*, "Rapid Deamination of Cyclobutane Pyrimidine Dimer Photoproducts at TCG Sites in a Translationally and Rotationally Positioned Nucleosome *in vivo*", *J. Biological Chemistry*, **290**, 26597-609 (2015).



ASSOCIATE PROFESSOR
DIRECTOR OF GRADUATE STUDIES

Chemical Biology and Medicinal Chemistry

Timothy A. Wencewicz

Postdoc, Harvard Medical School (2011-13); Ph.D., University of Notre Dame (2011); B.S., Southeast Missouri State University (2006).

Sloan Research Fellowship (2018); Cottrell Scholar Award (2017); NSF CAREER Award (2017); ACS Infectious Diseases Young Investigator Award (2016); ACS Division of Biological Chemistry Travel Award (2015); Oak Ridge Associated Ralph E. Powe Junior Faculty Enhancement Award (2014).

Antibiotic Drug Discovery. Infectious diseases continue to be a leading cause of death worldwide and the rapid development of bacterial resistance to current antibiotic chemotherapies is one of the world's most urgent health problems. Stepping up to this challenge, our lab is dedicated to the discovery of new antibacterial scaffolds and drug delivery systems that act against underexploited biological targets and overcome known resistance mechanisms. Our inspiration for new antibiotic therapeutics comes from structurally diverse microbial natural products, "Nature's Medicine", and relies on a coordinated effort of interdisciplinary approaches (organic synthesis, enzymology, spectroscopy, molecular biology, microbiology) to establish medicinal chemistry programs around unique, and sometimes complex, natural product molecular scaffolds.

Natural Product Biosynthesis. Nature has spent millions of years perfecting the chemistry to assemble infinitely complex molecular scaffolds found in secondary metabolites (natural products), primarily using biological catalysts (enzymes). Our lab is spending time to elucidate the timing and mechanism of biosynthetic enzymes involved in the assembly of medicinally important natural product antibiotics. We are particularly interested in learning how Nature biosynthesizes and stabilizes highly strained and reactive functional groups within molecular scaffolds, such as the hydroxy- β -lactam ring found in Tabtoxin ($T\beta L$ -Thr) produced by plant pathogenic species of *Pseudomonas syringae*. A "reactive" functional group often plays a key role in the molecule's mechanism of action, as discussed below.

Mechanism-Based Enzyme Inhibitors. Natural product scaffolds are highly evolved to bind a biological protein target with exquisite potency. Unique subsets of natural products possess latent reactivity that is realized only within the confines of its biological target and often results in the formation of a covalent enzyme-inhibitor complex. These types of molecules are often referred to as "Mechanism-Based Inhibitors" and can offer many therapeutic advantages (lower dosing and longer target dwell times). Our lab will elucidate the molecular mechanism of enzyme inhibition of naturally occurring mechanism-based enzyme inhibitors and exploit this knowledge to design and synthesize more effective synthetic inhibitors. We are interested in developing Tabtoxinine- β -Lactam ($T\beta L$) as a potent mechanism-based inhibitor of the enzyme Glutamine Synthetase to treat multidrug resistant *Mycobacterium tuberculosis* infections.

Targeted Drug Delivery Across Bacterial Membranes. Another attractive feature of developing natural products as antibacterial agents is that scaffold evolution during heated microbial molecular warfare created molecules with the ideal physiochemical properties for crossing bacterial cell membranes, a hurdle that frequently leads to the failure of new antibiotic compounds. Such is the case for Tabtoxin, a "Trojan Horse" dipeptide prodrug which enters cells via dipeptide permeases and liberates the $T\beta L$ warhead after cleavage by a dipeptidase. Some molecules even hijack energy-dependent active transport systems to cross the formidable bacterial cell wall. An example is the sideromycin natural products (siderophore-antibiotic conjugates) that utilize bacterial iron transport systems to smuggle antibiotic cargo across bacterial membranes. Our lab is characterizing how these natural drug delivery systems function in order to design and synthesize improved systems with sophisticated molecular linkers between the delivery vector and the drug that release the antibiotic payload in a microbe-triggered fashion.

Selected Publications

- T.J. Bohac, L. Fang, V.S. Banas, D.E. Giblin, and T.A. Wencewicz, "Synthetic Mimics of Native Siderophores Disrupt Iron Trafficking in *Acinetobacter baumannii*." *ACS Infect. Dis.*, **7**, 2138-51 (2021).
- N.P. Endicott, G.S.M. Rivera, J. Yang, and T.A. Wencewicz*, "Emergence of Ferrichelatase Activity in a Siderophore-Binding Protein Supports an Iron Shuttle in Bacteria." *ACS Central Science*, **6**, 493-506 (2020).
- D.F. Kreitler, E.M. Gemmell, J.E. Schaffer, T.A. Wencewicz*, and A.M. Gulick*, "The Structural Basis of N-Acyl-alpha-amino-beta-lactone Formation Catalyzed by a Nonribosomal Peptide Synthetase." *Nature Communications*, **10**, 3432 (2019).
- J.L. Markley, L. Fang, A.J. Gasparrini, C.T. Symister, H. Kumar, N.H. Tolia*, G. Dantas*, and T.A. Wencewicz*, "Semisynthetic Analogues of Anhydrotetracycline as Inhibitors of Tetracycline Ductuctase Enzymes." *ACS Infectious Diseases*, **5**, 618-633 (2019).

C.T. Walsh and T.A. Wencewicz, "Antibiotics: Challenges, Mechanisms, Opportunities." January 2016, ASM Press, Washington DC, USA.

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ASSISTANT PROFESSOR

Computational and Theoretical Materials Robert Wexler



Postdoctoral Fellow, Princeton University (2019-22); Ph.D. University of Pennsylvania (2019);
B.S., Drexel University (2013)

Award for Excellence in Chemistry Graduate Research, UPenn, Dept. of Chemistry (2017); Dept. Fellowship, UPenn, Dept. of Chemistry, (2016); Teaching Assistant Award, UPenn, Dept. of Chemistry (2015); William Fontaine Fellowship, UPenn, Dept. of Chemistry (2013); Senior First Honors, Drexel Univ., Dept. of Chemistry (2013); HyperCube Scholar Award, Drexel Univ., Dept. of Chemistry (2013); American Institute of Chemists Baccalaureate Award, Drexel Univ., Dept. of Chemistry (2013).

The Wexler Group is focused on theoretical innovation for renewable energy and environmental applications, with an emphasis on the development of computational methods for the more realistic modeling of interfacial phenomena in heterogeneous electrocatalysis, solar energy conversion, and ferroelectric environmental energy harvesting.

As the damages associated with climate change intensify in the coming years, it will become increasingly more important to focus on sustainable energy and environmental remediation. Computational materials chemistry coupled with data science and machine learning (ML) has the potential to revolutionize the industries responsible for these damages by alleviating their reliance on fossil fuels, precious metals, and toxic elements. Inspired by this potential, the Wexler Group focuses on solving grand challenges in energy and environment by designing and developing next-generation technologies for water splitting, carbon dioxide utilization, solar energy conversion, and environmental energy harvesting. Solving these challenges in catalysis, solar power, and transduction will require improvements in the way that surfaces are currently modeled, which can be achieved via next-generation multiscale methods for ab initio thermodynamics that combine our expertise in first-principles quantum mechanics calculations (for obtaining electronic precision), Monte Carlo (MC) and molecular dynamics simulations (for establishing macroscopic understanding), and data science/ML (for extracting insights).

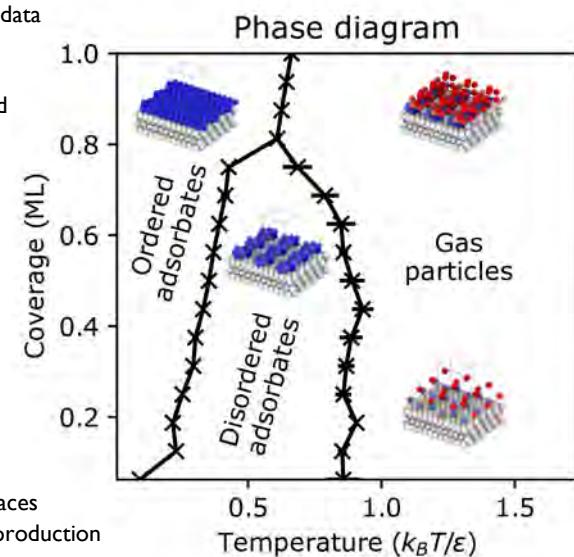
More broadly, our research can be subdivided into four distinct directions that address these challenges from different angles:

1. To develop state-of-the-art computational techniques for the realistic modeling of surfaces
2. To provide fundamental understanding and design principles for sustainable hydrogen production and carbon dioxide conversion
3. To improve solar-cell efficiency via chemical modification and interfacial engineering
4. To create efficient ML tools for the accurate simulation and rational design of ferroelectric energy harvesters

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Selected Publications

- R.B. Wexler, G.S. Gautam, R.T. Bell, S. Shulda, N.A. Strange, J.A. Trindell, J.D. Sugar, E. Nygren, S. Sainio, A.H. McDaniel, D. Ginley, E.A. Carter, and E.B. Stechel, "Delocalized Reduction of A-Site Ce in Ca-Ce-Ti-Mn Oxide Perovskites for Solar Thermochemical Applications", *Energy Environ. Sci.*, (2023).
- R.B. Wexler and E.A. Carter, "Oxygen-Chlorine Chemisorption Scaling for Seawater Electrolysis on Transition Metals: The Role of Redox", *Adv. Theory Simul.*, 2200592 (2022).
- R.B. Wexler, G.S. Gautam, E.B. Stechel, and E.A. Carter, "Factors Governing Oxygen Vacancy Formation in Oxide Perovskites", *J. Am. Chem. Soc.*, 143, 13212–27 (2021).
- R.B. Wexler, G.S. Gautam, and E.A. Carter, "Optimizing Kesterite Solar Cells from Cu₂ZnSnS₄ to Cu₂CdGe(S,Se)₄", *J. Mater. Chem. A*, 9, 9882–97 (2021).
- R.B. Wexler, Y. Qi, and A.M. Rappe, "Sr-Induced Dipole Scatter in Ba_xSr_{1-x}TiO₃: Insights from a Transferable-Bond Valence-Based Interatomic Potential", *Phys. Rev. B*, 100, 174109 (2019).
- R.B. Wexler, T. Qiu, and A.M. Rappe, "Automatic Prediction of Surface Phase Diagrams Using Ab Initio Grand Canonical Monte Carlo", *J. Phys. Chem. C*, 123, 2321–8 (2019).
- R.B. Wexler, J.M.P. Martirez, and A.M. Rappe, "Chemical Pressure-Driven Enhancement of the Hydrogen Evolving Activity of Ni₂P from Nonmetal Surface Doping Interpreted via Machine Learning", *J. Am. Chem. Soc.*, 140, 4678–83 (2018).