

Jackson Lab Manual

(Updated 6/04/25)

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I. INTRODUCTION

Mission Statement: We integrate AI with physics-based molecular modeling to study electronic processes in organic materials. We pride ourselves on having a supportive group culture.

What is our expertise? We are not a traditional theoretical chemistry group focusing in a single methodological area (e.g. electronic structure, quantum dynamics, or statistical mechanics) – the problems we work on are highly interdisciplinary and will expose group members to an array of theoretical and computational techniques. With this said, our core expertise is in three areas: multiscale molecular modeling, AI for chemistry and materials, and soft materials chemistry.

Group Culture: The Jackson group is committed to maintaining a positive research and learning environment based on open communication, mutual respect, and non-discrimination. The Jackson group will not discriminate based on race, sex, age, gender, economic class, disability, veteran status, religion, sexual orientation, color, or national origin.

II. WORKPLACE EXPECTATIONS

Where I Want You to Be at the End of Your Ph.D

- You are a legitimate expert in a scientific or technical topic.
- You can define an original and meaningful scientific question.
- You can define and execute a research plan to address that question.
- You can generate from that research an accepted research product (e.g. publication, patent) with little to no guidance in a 1-2 year time frame. This includes:
 - Writing a complete paper draft with little-to-no input or guidance.
 - Making effective slide sets and oral presentations with little-to-no input or guidance.
- You possess strong coding ability in at least one language (e.g. Python, C++, Fortran).
- You follow the 48-7 rule. You try a new task for at least 48 hours before asking for assistance, but do not wait longer than a week to ask for assistance if you cannot make any progress.
- You know how to give criticism.
- You can take hard criticism without taking it personally.
- You are friendly when approached by others for help or feedback.
- You are professional, arrogance-free, and not condescending.

Responsibilities of the PI: The goal of the Ph.D program is to train you to have the above skills and attributes by the conclusion of your Ph.D. This requires substantial efforts on both your part and my own. My plan is to mentor you closely until you reach your candidacy exam (year 3). Following your candidacy, you will take on more independence and develop and execute your own scientific ideas within the context

of your project(s). I plan to be more hands-off as you progress further through your Ph.D. – you have the fundamentals, you have demonstrated technical competency, and now the goal is to develop independence in your research. In the last year of your Ph.D., my role will become that of a delegator – I will be assigning you projects, trusting in your technical competency and ability to creatively problem solve, and becoming your advocate as you progress towards your next career stage. Whatever future career (e.g industry, academia, government) you are interested in, I will support you to the absolute best of my ability.

How much am I expected to work? The focus is on progress in your project(s) rather than the number of hours worked. A critical part of graduate school is developing your own effective time management habits that lead to productivity. On *average*, I have observed that people that work ~50 hours/week are successful. I **discourage** working more than 60 hours per week to avoid burnout. I encourage you to develop a schedule that allows you to regularly interact with your lab mates in the lab – you will learn as much from them as you do from anybody else in graduate school.

My schedule: I plan to be in the office or actively monitoring my email and the group Teams channel 8 am - 6 pm daily. I generally do not answer emails between the hours of 9 pm and 8 am.

What are the hard requirements for a Ph.D in the Jackson Lab?

- **1st year** – 5 graduate level courses with at least a 3.0: CHEM540 (Quantum Mechanics) and CHEM544 (Statistical Mechanics) are required. The other three can be any graduate level courses across UIUC. (departmental requirement). For our group I strongly recommend you take CHEM452: Data Science for Chemistry & Engineering as one of these courses.
- **1st year** – Two semesters of teaching assistantship (departmental requirement).
- **2nd year** – Literature seminar (CHEM545) (departmental requirement).
- **3rd year** – Oral Prelim Exam (1-2 hours) and Report (10 pages) to thesis committee on research to-date (departmental requirement).
- **4th year** – Original Research Proposal (departmental requirement)
- **5th year - Thesis Defense** (departmental requirement)
 - If you would like to get a position in industry after you graduate, I **strongly encourage** you to do an internship, preferably in the summer before your 5th year.
 - Presentation at a professional conference (Jackson Lab requirement)
 - A minimum of three submitted 1st author publications (Jackson Lab requirement)

How do I make sure I have a successful Ph.D.?

Rule 1: Take ownership of your project. Know the background information and caveats of your research thoroughly. Frequently re-evaluate where you think your project should be headed and devise potential paths for moving forward in those directions. I encourage you to communicate these ideas with me so that I can give you feedback – it is more than likely that some of your ideas will be fantastic avenues to pursue and I want you working on ideas related to your project that **you** came up with.

Rule 2: Learn from others and understand what you are learning. It's OK to initially use software packages and theories as black boxes for exploratory calculations, but you will not be publishing any results until you understand the techniques that you are using to generate data.

Rule 3: Get the help you need both within the group and outside of it: group meetings, seminars, other lab members, your committee, and other faculty in the department. There is an expert at UIUC in almost any topic of interest – take advantage of that.

Rule 4: Don't lose yourself in your project. Science is a constant exercise in finding the deepest minimum in a potential energy surface that provides the best rewards. Digging down into your project from a single perspective is key to making advancements – however, don't forget to broadly educate yourself (seminars,

literature) in areas outside of your immediate expertise. The history of science (theory in particular) is often one of people taking ideas from other fields and applying them to their interest areas. Exposing yourself to many different ideas is a key element of making progress in your own specialization.

Rule 5: Learn how to train people. A Ph.D. enables one to lead research teams (industry, government, academia) – you can't lead research teams without a Ph.D. Take the time to show others within the group how to do things (undergraduates, graduates, postdocs, me!).

Time away from the Laboratory:

- *Vacation policy:* 30 total vacation days (note: major holidays such as Christmas, New Years and University holidays are to be counted as vacation days). Students can use these days whenever they want. If you will be absent for 1-2 days, please give me a day's notice (if possible). Please provide several weeks' notice about an upcoming vacation that lasts more than one week (this is to ensure that if I need a result provided for a grant or a poster presented during your absence, I can adapt various members' schedules to accommodate this in advance).
- *Sick days:* If illness or mental health are interfering with your research, time off is expected and this does not count as vacation days. Please do not come to lab if you have cold, flu, or covid-like symptoms. If overall health is significantly affecting your research progress, a leave of absence should be discussed with the PI.
- *Mental health:* I am passionate about student mental health. Should you be suffering from mental health issues, please let me know and I will be happy to work with you to develop a more accommodating schedule. If you feel that you need a mental health day, please take one and let me or someone in the group know that you will be doing so. Also, please avail yourself of the University's mental health resources (<https://www.counselingcenter.illinois.edu>).
- *Emergency situations:* Family emergencies are covered as the same policy of illness. Please notify me if you will be out for a family emergency.
- *International students:* It is understood that international students may take less frequent but more extended vacation time, often in the summer.
- *Adverse weather:* If classes are cancelled, or the temperature is below 10 degrees Fahrenheit, students may elect to work from home.
- *Conferences:* Do not count as days off.
- *Job Interviews:* Do not count as days off.
- If you are considering maternity/paternity leave, please contact me directly to develop a schedule that supports you and is consistent with University policies.

External Funding: When a graduate student is accepted into the group, I maintain full responsibility for funding that person through either RA or TA appointments throughout the course of their Ph.D., consistent with departmental standards. I strongly encourage any students interested in applying for external funding opportunities (NSF GRFP, DPE CSGF, DOD NDSEG, etc) to mention this interest to me so that we can work towards creating a strong application.

When a postdoctoral researcher is accepted into the group, the term of their appointment and potential for renewal will be negotiated and made clear in the offer letter. If current or potential postdoctoral researchers are interested in applying for an external fellowship, they should contact me directly by email to discuss such opportunities.

Rules for One-on-One Research Meetings: I expect you to present a slide set that (i) covers the progress you have made, (ii) describes any challenges that you have faced, and (iii) outlines what you are working to accomplish before our next meeting. I will provide feedback on your progress, provide advice for overcoming research challenges, and critique your proposed work.

Communication is Key: The best way that both you and I can get the most out of your Ph.D. is by having open lines of communication. I will do my best to constantly communicate my thoughts and expectations to you, and you should do the same for me. Small regular adjustments are much more effective (and less stressful) than a single massive course correction down the road. I am a firm believer that happy and motivated people do the most creative science, and communication is critical to this.

Expectation of Conduct: Students are expected to uphold the highest level of ethical conduct in accordance with the policies of the University of Illinois. Unethical conduct such as fabrication of results can seriously jeopardize one's career and goes against what we stand for as scientists.

The Jackson group is committed to maintain a safe and welcoming environment for all, regardless of race, gender, sexual orientation, disability, physical appearance, religion, and other identifiers. All students are expected to maintain an environment free from harassment and discrimination, in accordance with the policies set out by the University of Illinois. If you witness, or are the target of, harassment or discrimination, please consider reporting it to Prof. Jackson, to the Assistant Director of Graduate Diversity & Program Climate, or to your Title IX coordinator.

III. PERSONAL WELL-BEING

Happiness: You are here to do a Ph.D. at one of the top research institutions in the world. You were admitted under the premise that becoming an outstanding and productive scientist is what you want to do with your life. I am operating under the assumption that you are passionate about doing the work necessary to receive a Ph.D., and that you are independently driven to accomplish this goal. My job is to help you achieve this goal via training and mentorship within my laboratory. With that said, life is more than your pursuit of a Ph.D. You should work hard, be proud of what you accomplish, and push yourself intellectually and creatively. However, nothing comes before your health and wellness. I firmly believe that happy people do the best and most creative science, and I strongly encourage you to cultivate personal health and wellness in your life.

Group Care Activities:

- If you notice a person in the group is out for several days, check in with that person (not calling them out to others).
- No judgement, just checking in (e.g. "Just wanted to make sure you are doing okay" or "Do you need help with anything?")
- Going to the doctor, going to counseling, working out, going to yoga, going to a meditation class, going for a walk – these are all activities that are strongly encouraged. There is no need to report these activities. Of course, we agree as a group to not abuse this policy.
- [RSO database](https://union.illinois.edu/get-involved/office-of-registered-organizations) (<https://union.illinois.edu/get-involved/office-of-registered-organizations>)
- [ARC group fitness schedule](https://campusrec.illinois.edu/programs/group-fitness/group-fitness-class-schedule/) (<https://campusrec.illinois.edu/programs/group-fitness/group-fitness-class-schedule/>)
- [Counseling Center](https://counselingcenter.illinois.edu/) (<https://counselingcenter.illinois.edu/>)
- [McKinley Health Center](https://mckinley.illinois.edu/) (<https://mckinley.illinois.edu/>)
- [Women's Resource Center](https://oiir.illinois.edu/womens-center) (<https://oiir.illinois.edu/womens-center>)
- [Cultural Houses](https://oiir.illinois.edu/our-centers) (<https://oiir.illinois.edu/our-centers>)

IV. GROUP OPERATIONS

Our group runs an active Teams channel, and every member should join this channel immediately upon joining the group. It is best to use this for as much communication with group members (and myself) as possible, research or otherwise. We also have a group email listserv – please ask Nick or a group member to be added to this. Also, please ask to be added to our group Box folder that contains a wealth of resources

for science and general training within the group. Finally, information about cluster usage within the group can be located found here: scruggs.readthedocs.io

We have a weekly group meeting, the time of which changes each semester to adapt to the group's schedules. One person per week presents slides for ~45 minutes, alternating between research and literature talks. The literature article should be approved by me and distributed to the group at least two days prior to the presentation. If you have any questions about the content of either talk, please contact me or a senior group member for more information. Attendance at group meeting is mandatory.

V. CONFLICT RESOLUTION

Authorship: Authorship should be discussed at the beginning of projects with all potential authors and should be agreed upon unanimously. Frequently, authorship can change as projects progress, but any changes should be discussed with all authors. The order of authorship is impacted by many factors, but the final order should be determined by PI. Students cannot promise authorship orders (e.g., "If you do this, you'll be second author.")

Student-to-Student Conflicts: Start person-to-person – attempt to resolve the conflict in a gentle, non-accusatory tone. If the conflict escalates beyond what can be solved between the people involved, the conflict should be brought to Nick's attention. If required, Nick will contact Justin M. Brown in the Office for Student Conflict Resolution to help resolve the matter. If the conflict is threatening to one's life, call 911 and then notify Nick. All ethics and scientific integrity issues should be reported to Nick. Note that any discrimination or excessive rudeness within the group should be brought to Nick's attention and addressed as potential grounds for exiting the group.

Student-to-PI Conflicts: We recognize that there is a power difference involved in the resolution of such a conflict. It is preferred that a student would first manage the conflict informally in-house without involving administrators (if possible) via an email to Nick, another graduate student's mediation, or a meeting with Nick. Students should let Nick know if they feel that his response was inadequate and could do so via email. If the student still feels that the conflict has not been resolved, the student should let Nick know and address the issue with another mediator. Mediators/resources for graduate students include the departmental Assistant Director of Diversity and Climate, the Director of Graduate Studies, and the Faculty Staff Assistance Office.

Group Conflict: To avoid group issues, group members should clean up after themselves ASAP, particularly within shared spaces. Group clusters should not be abused, and basic cluster etiquette should be obeyed.

VI. EXIT POLICIES

Graduation Policies:

When a group member graduates, with a PhD or as a masters, the group member's contributions should be celebrated in a group event. The group event may be a shared meal, a potluck, a board games party or any other appropriate activity.

Regardless of how a group member exits the group, steps should be taken with cooperation from the departing group member to ensure that any useful skills or knowledge developed by said group member will remain available to the group.

- All manuscripts to be completed should be agreed upon by both Nick and the group member, prior to leaving.
- Before the group member physically leaves (ideally as soon as an exit is planned), the supervisor, the departing group member and any in house collaborator (e.g. co-authors on papers) should meet and agree on what needs to be documented in writing and what needs to be passed on in training.
- To ensure completeness, the written documents should be read and understood by the professor and continuing group members.

Types of Potential Jobs and Where to Look:

The skillsets developed within this group are in line with jobs in several areas. The information provided below is not exhaustive, and merely represents examples to use as starting points:

- *Chemical and Materials companies:* 3M, IBM, Intel, Applied Materials, Solvay, Applied Materials, PPG, Dow-Dupont, Corning.
- *Biotech and Pharmaceuticals:* Lilly, D.E. Shaw, Zapata Computing, Silicon Therapeutics, Illumina, Pfizer, AstraZeneca. There are a thousand start-ups in this area as well.
- *Scientific Software Companies:* Schrodinger, Entos.
- *Data Science and Software Engineering:* Google, Microsoft, Facebook are the usual culprits, but there are thousands of others, including start-ups.
- *Consulting Firms:* Institute for Defense Analyses, Exponent, McKinsey, Boston.
- *Government:* Program managers, analysts, and consultants at NSF, DOE, DOD, EPA.
- *Patent Agent at Law Firms*
- *Teaching Focused Professor or Lecturer*
- *Post-docs in Academia:* Ask Nick for more details. Any university.
- *Post-docs in National Laboratories:* Ask Nick for more details. Argonne, Oak Ridge, Lawrence Berkeley, Sandia, Pacific Northwest National Laboratory, Los Alamos, Lawrence Livermore, Brookhaven, Ames, National Renewable Energy Laboratory, Naval Research Laboratory, US Army Research Laboratory, US Air Force Research Laboratory.

Leaving the Group (Non-Ph.D. Graduation):

If graduating with a PhD is no longer an option or if a student no longer intends to continue in the PhD program, the student may consider graduating with a master's degree.

- The requirements for a master's degree by coursework are enumerated in Section 4.3.1 of the Dept. of Chemistry Graduate Manual.
- The coursework and documentation requirements for a thesis master's degree are enumerated in Section 4.3.2 of the Dept. of Chemistry Graduate Manual. Research requirements should be determined through discussion between the student and the professor, possibly in consultation with the program coordinator.

If a student wishes to switch to a different research group, the student should follow the procedures described in Section 5.2.14 of the Dept. of Chemistry Graduate Manual. In addition, the student should ensure continuity of skills or knowledge (see point two) before exiting the group to the best of the student's ability. If the professor finds a student's work performance unsatisfactory, the professor must provide a written, detailed account of 1) how the student is not meeting expectations and 2) what the student needs to change or start doing to meet expectations. Presenting this written account to the student will initiate a

90-day probationary period for the student to implement these changes. This probationary period is distinct from the post-termination 30-day period described in Section 5.2.14 of the Dept. of Chemistry Graduate Manual.

After this 90-day probationary period, if the professor wishes to seek the exit of a student from the group, the professor should notify the student in writing of the causes for which their exit is sought. The professor should proceed as described in Section 5.2.14 of the Dept. of Chemistry Graduate Manual.