

ATOMS LAB EXPECTATIONS AND GUIDELINES

The goal of this document is to clarify the roles and expectations for me, the advisor, and you, a new member of the group.

The overarching goal in the ATOMS Lab is to train amazing researchers who bring valuable skills to industry, academia, and national research labs. Technical skills include writing code, working with supercomputers, running simulations, analyzing data, and solving chemical engineering problems. However, *even more valuable* skills are so-called transferrable skills, such as communication, cooperation, professional networking, time management, personal organization, project management, reading the literature, giving presentations, and writing – when you practice excellence in these areas, you make the world a better place, in whatever role you pursue after your time in the ATOMS Lab. I hope you'll enjoy working with us, and that you'll gain the skills needed to grow into an independent researcher.

Along the way, we aim to address exciting research questions, especially around figuring out how to build artificial agents that comprehend and solve problems in chemical theory, to eventually accelerate scientific discovery and gain molecular-scale insights on processes in the environment that enable new solutions for cleaner air and water. However, research does not contribute to the scientific knowledge until it becomes a peer-reviewed publication. Peer-reviewed publication is also the primary mechanism we use to achieve personal and technical growth. Through the research, thinking, and interpersonal interaction required to write these papers, students grow, learn, and mature. Thus, all the work you do is eventually headed toward publication. Undergraduate students are expected to contribute to a paper before graduating. Masters students are expected to lead-author or significantly contribute to a journal article before graduating. PhD students are expected to lead-author 2-3 papers before they graduate.

We also share our research via oral presentations at virtual, local, and national conferences, and I will help you develop the skills to do this effectively. I will also try to raise money to help offset the costs of attendance. I welcome your own efforts of funding your attendance, as well, through departmental and university funds, scholarships from the societies sponsoring the meeting, and outside groups. I hope between my funds and your ability to raise money from these sources, graduate students will be able to present at one meeting/year and undergraduate students will be ready to present by their senior year.

Research is fundamentally different than nearly every other academic activity you've done. This is because research, by definition, involves developing understanding of *new* problems. Because it's never been done before, it may not be possible to do at all! This contrasts with every homework or test problem you've ever solved – these have known answers. Furthermore, interesting problems tend to get solved by other researchers, *unless they're really hard to solve*. The implication is that success requires a concentrated studying, time, and energy. You'll need to learn enough about a problem to understand what other researchers have tried, and then (often creatively) propose something new *and* implement it, and everything must be done well enough so that peers are impressed, as well.

Because I and current members of the ATOMS Lab are going to invest in you, we have a reasonable expectation that you demonstrate two things: (1) Ability and (2) Motivation. Ability means that you're able to learn, solve problems, read and write code, analyze results, present, etc. as you've already demonstrated through your course work. Motivation means you're enthusiastic about, and committed to, your project. Motivation will typically manifest itself by you making lab work a reasonable priority in your schedule, by coming to meetings and by spending consistent and significant amounts of time on your project.

While the specifics of this document are oriented toward undergraduate researchers, the spirit of the document also applies to graduate and post-doctoral researchers.

Both faculty supervisor and student have read and agreed upon the following conditions:

SUPERVISOR RESPONSIBILITIES

I serve as an **advisor** in your research, offering guidance and advice. Together we will design a research project tailored to your interests, but that still meets the objectives of the funding (grant) that supports your work. As your advisor, you can expect me to:

- Help you set reasonable goals and create a plan to achieve them
- Be available for regular and informal meetings
- Teach you what I can about the techniques needed for your research
- Review your research products, providing constructive feedback on the quality and progress of your work towards your goals
- Promote you and your work to the University and the larger scientific community
- Teach you about how to best present your work in formal talks and in publications
- Support you in your professional development activities
- Help you write scholarship applications, letters of recommendation, find great jobs, etc.
- Write grants to support you and future members of the ATOMS Lab
- Give you an opportunity to give feedback on my role as an advisor

STUDENT RESPONSIBILITIES

Student responsibilities: Scientific research is a labor-intensive enterprise that demands a high level of personal commitment, time, effort, and collegial participation in the functioning of the lab. The student promises to dedicate the necessary time and effort to complete the project. Undergraduate students are normally expected to work approximately 10 hours per week during the semester and full time during January and the summer. Students agree to submit written material that requires feedback no later than 14 days before a deadline. Students should conduct themselves in an appropriate and ethical manner at all time when dealing with other students, employees, faculty, and research participants.

Group meetings: Student agrees to attend ATOMS Lab group meetings. Students will present their research at these meetings. Prior to journal club meetings, student agrees to read the assigned paper. Every attendee at group meeting is expected to ask one question.

Reports and individual meetings: Student and advisor agree to meet at least twice a month for an individual meeting. Student agrees to write a weekly report to share with the advisor prior to meeting, which will include the weekly goals, data from the prior week's work, and questions for the advisor. This becomes a "living document" that is added to each week.

Networking and professional development: Networking, or "making professional friends," is critical for your professional success. Every member of the ATOMS Lab must network with one new person each term (Fall, Spring, Summer). We will provide training (it can be daunting for those who haven't done it before!), but you are responsible for cultivating your own professional network. Students are also encouraged to become members of professional societies relevant to their work.

Research proprietary: All new code and research data from the project are the property of UMBC. Dr. Josephson will determine the circumstances that the student and others may have future access to these code and data. When applicable, student agrees to sign a non-disclosure agreement regarding intellectual property.

Responsible Conduct of Research: Student commits to never lying or misrepresenting him/herself or data. Student further agrees to keep a comprehensive lab notebook (preferably electronic), which is the property of UMBC. Each year, every student will complete on-line Responsible Conduct of Research training.

Obtaining a degree: It is the student's responsibility to know the requirements for their program. Requirements can change frequently and are not standard across different degrees (e.g. Master's vs. Ph.D in ChemE or in CS). This information is often available from the department or program director, so please start there and direct questions of this kind towards that individual. If you are having trouble with a particular issue, please ask me for help.

Time: For the period academic year 2021-2022, student agrees to work an average of 10 hours/week. Prof. Josephson agrees to pay student for this period when funds are available.

I look forward to working with you!

Student name/date

Tyler R. Josephson/date

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Modified from and inspired by agreements by Amy Burgin, Mark Marten, and Jim Pfaendtner
