

Gruebele Group Manual

Updated 12/12/2020

1. Introduction

- Since 1992, the Gruebele group studies the dynamics of complex systems using theory, computation and experiment, with key instruments developed in-house. The research draws participants from chemistry, physics, biophysics, and biochemistry, although the short classical description would be a ‘physical chemistry research group.’ Our mission is to train scientists at all levels from undergraduate to staff scientist for careers in industry, government or academia, with the goal to create a diverse scientific workforce, while answering questions at the boundaries of the unknown.

2. Workplace Expectations

Responsibilities of the PI

- Martin’s overall role is to conceptualize research projects, to facilitate an inclusive environment, to provide regular advice to students, postdocs and staff on their projects, to secure funding so these projects can be carried out, and to participate in data analysis, paper writing, and presentation of results to the community at large. Others in the group also participate in these activities (in addition to their personal or collaborative projects) depending on experience.
 - o Students should expect to be assigned two to three projects of differing levels of difficulty to provide alternatives when one of the projects is moving slowly. In particular, Martin encourages computational/theory/data analysis projects in addition to experiments as they have more flexible time management.
 - o Martin is relatively hands-off in terms of advisory meetings, that is, except for a weekly group meeting, students can co-define what meeting schedules and updates suit them best. This is in recognition of different work styles that evolve as students progress towards scientific independence. A weekly meeting can be expected by any lab member who is interested in it, and students are encouraged to reach out, just as Martin will ask for meetings when he thinks it will be helpful.
 - o Martin should generally be able to schedule a meeting within a week, and of course immediately if the situation is urgent. During travel a phone- or internet-based meeting can still be expected.
 - o Martin obtains funding with the goal for students not to teach after their first year unless they wish to or the department asks for teaching expertise of an advanced student. The one year teaching load is contingent on funding availability, but Martin generally budgets and hires with this goal in mind and between 1992-2020, no student had to teach due to funding unavailability.
 - o Martin should advertise funding opportunities (e.g. Fellowships), conference opportunities, as well as job opportunities when appropriate. Likewise, he is available for career-related meetings if desired. A conference attendance per year is a minimum every lab member with at least a year of experience and new results can expect, and students can identify meetings or Martin will provide suggestions. Martin generally expects a talk or poster to be presented in order to cover conference costs, but sometimes meetings are attended as a networking and learning experience only.
 - o Martin should provide a fair assessment of co-authorship on publications, including first-co-authors, and consult with all authors on a paper to ensure that there is consensus on authorship based on the contributions from all the authors, in particular the important first- and co-first author positions. During manuscript preparation Martin will provide regular feedback on text and data analysis, while writing or doing analysis himself. It should typically take 1-2 months to write a paper once the key data has been collected.

Expectations of students

- Within reason, group members can define their own work hours, in recognition of different people’s different goals and situations (e.g. families). Productivity is judged by progress reports in individual

or group meetings, and includes research output (as our primary mission), but also other activities such as participation in outreach programs or student governance. Martin's experience is that group members putting in consistently below 50 hours/week have not fared as well as those putting in 50-60 hours a week; likewise, group members working for over 70 hours/week (against Martin's advice) have in some cases suffered burnout. The practical skill Martin values most is the development of independent research ability while working in a team, including the time management skills to maximize one's personal productivity. The personal skill Martin values the most is team-playing and compassion.

- Martin encourages students to apply for Fellowship opportunities, and more advanced students (typically 3^d year and up) can participate in grant writing beyond just basic information provision if they are interested.
- Postdocs typically have more experience, and are expected to participate in the guidance of graduate students and grant writing in addition to co-mentoring and collaborating with one or more graduate students. Likewise, advanced graduate students are expected to take first years 'under their wings' if the projects are related.
- Students on an RA or Fellowship are expected to dedicate their time mainly to their research projects.
- As a 50% TA, a graduate student is expected to split their time roughly 20 hours/week TA, the rest on research, outreach and other activities.
- Undergraduate students will always be assigned a graduate or postdoc mentor, and are expected to provide clear information on their availability, which needs to be in 5+ hour blocks in order to accomplish work in the lab. Projects may be for credit during the semester (1 hour credit per 4 hours of lab work, as is typical of lab classes), or an hourly stipend *or* credit during the summer). Martin will always consult with potential mentors before they are asked to take on a mentoring task.
- All students are expected to complete safety training, ethics training, and other such modalities required by the department, college, campus or State in a timely fashion.
- Lab members are expected to collaborate to keep the lab safe and clean, and maintain instruments or complete other tasks assigned to specific responsible parties in a timely fashion.

Time away from the laboratory

- The Gruebele lab follows the Department of Chemistry and Graduate College policies on personal time off (see links in bibliography), mental health leave or family leave. Students should inform Martin of intended time off with timely notice to allow smooth operation of the group. As a rule of thumb, the advance notice should be comparable or longer than the duration of time off requested.
- Time off will be given for emergencies which require an unexpected absence from lab. To the extent possible, students are still expected to adhere within reason to the cumulative annual time-off guidelines set forth by Department and Graduate College.
- Martin allows such time off to accumulate: someone (e.g. an international student) who cannot take time off regularly can do so more rarely for longer periods (within the cumulative time-off guidelines), as long as sufficient notice is given. Students are encouraged to take potential work with them on trips in case delays (e.g. visa) arise, and such remote work fully counts as regular research work. Students are encouraged to take their 'time off' completely off unless such delays arise.
- The group honors the diversity of holidays and any other reasons why time off is personalized.

3. Expectations of progress towards degree

Feedback mechanisms

- A significant contributor to stress in graduate school is a feeling of not knowing where one stands. Martin should provide at least annual, and if warranted more frequent, feedback on this topic, as work interests of students develop, to best adapt projects to interests. The discussion can go through formal

written mechanisms (such as the departmental online review), or preferably thorough personal discussion allowing enough time (at least an hour).

- Martin monitors progress mainly by two mechanisms: a research group meeting by each group member twice a year, and informal (i.e. not necessarily regularly scheduled) one-on-one or small meetings with students or postdocs. Group members can request these meetings, or Martin will generally request them at various intervals to keep up-to-date on progress and offer advice.

Departmental requirements

- Literature Seminar:
 - o Students should prepare a cohesive literature seminar; they can involve the group as a test audience, but this is not formalized in the Gruebele group because the lit seminar is a class with its own built-in audience. Martin and other group members are expected to attend the final seminar unless a time conflict really prevents it.
 - o Preparation of a lit seminar will be similarly time consuming as preparation of a poster or talk for a conference, i.e. a cumulative 20 hours outside of class time as an average effort.
- Prelim exam:
 - o The prelim exam is the most critical exam of a graduate career, and thus likely the most stressful.
 - o The committee is selected in consultation with Martin, but the student has the final word. Students are encouraged to meet regularly (e.g. once a semester) with committee members about their work. Getting to know at least one or two committee members well is useful for many things, such as recommendation letters.
 - o As a rule, students who have a publication submitted or ready as a preprint are in excellent shape for their prelim, and should focus on a brief review of that past work and a longer review of the future work needed to complete the PhD. Students who struggle will have meetings with Martin for him to point out what can help. Indeed, if Martin thinks a student is not likely to pass the prelim (which has happened a few times between 1992 and 2020), he will discuss this with the student months ahead and explore alternative options; the final decision whether to move ahead with the prelim remains in the student's hands.
 - o It is not unusual to spend over 50 cumulative hours during the prelim semester specifically on the prelim aside from research (e.g. lit searches, background reading, slide and talk preparation).
 - o Students must give the talk to the group a few weeks before the exam for internal feedback. Martin's best advice is never to put any image, equation or phrase on a slide that the examinee cannot discuss at least one level deeper. Of course additional practice talks with group members or others can also be scheduled.
 - o It is important to turn in prelim information and paper in a timely fashion to the committee. Martin is happy to review the paper if given a draft several days before the committee deadline, but the paper reflects a student's own views of the subject and will not be extensively edited by Martin.
- ORP:
 - o The ORP format is now a proposal + presentation across most areas of the department.
 - o Students should spend a time about twice that of the lit seminar, and in particular make sure they can recall the background literature and salient facts during the ORP presentation, which should be ca. 20 slides long.
 - o Martin will be happy to comment on the ORP slides and proposal if he gets them several days before they are due to the committee.
- Graduation:
 - o The historical average time to graduation in the Gruebele group is 5 years, and has ranged from 4 to 7 years, the latter for a GK-12 Fellow who took 5 years in lab and two years for the teacher program that is part of GK-12.
 - o Generally, Martin will discuss graduation timing and prospects with students towards the beginning of their fourth year, and regularly follow up on it, just as students can request such a discussion.

- Typically, two first author publications from different projects or different aspects of a project are the minimum for a strong PhD thesis, although as few as one and as many as a dozen first-author publications have resulted from theses between 1992 and 2021.
- Work on the thesis document is expected to consume about half of a student's time in the last semester, in addition to paper writing and wrap-up on projects that are near completion, as well as training other students on projects to be handed over.
- The thesis format should be in conformance with Graduate College requirements. Martin has no additional requirements on length, placement of figures, etc., as this document reflects the student's intellectual output, not a joint effort like a publication. The document should be delivered to Martin at least a week before the thesis committee deadline for feedback, and a 40 minute presentation highlighting the most important aspects for a general audience should be prepared, and test-driven with the group.

4. Lab resources/general policies

Meetings

- Group meetings will be scheduled during the work week allowing as many to attend as possible. Attendance is always expected unless there is a severe scheduling conflict or emergency. Duration is usually 1.5 hours, and the focus of group meetings is research results or recent publications achieved during the last semester. Beginning students may also review relevant literature. Due to very diverse interests in the group, a general introduction and review of ~5 slides is encouraged, but group meetings should not be too repetitive of old material.
- Students are expected to attend seminars. At a minimum they should attend the weekly seminar of their area and its annual major invited lecture(s). Students may also attend other seminars of their choosing. Generally, 2±1 seminars a week is a good number to attend on average, although student interests may lead to more or less than that average in any given week.
- Prelim and PhD, as well as conference presentations, will be handled either as group meetings or *ad hoc* meetings set by the student for other group members. Attendance at *ad hoc* meetings is not required, but encouraged to provide support and feedback, particularly from group members doing related work.

Purchasing

- Pre-approval of orders is generally not required as Martin reviews and approves all orders for the group. However, for orders exceeding \$500 it is nice to inform Martin for the need separately; this could be done in person, or via an email when the order is being submitted.

Data/sample management

- All group members must keep a dated lab notebook, which may be manual or electronic. Incorrect entries should never be ripped out or defaced, but rather just neatly crossed out. Notebooks with detachable pages are unacceptable, as are electronic methods without a trace history. Graduating students must leave their notebooks and a drive with all data, although they can take copies with them if they wish. All group members must back up their data regularly and in multiple locations (e.g. on Box, lab computer, personal computer, thumb drive, etc.) in case a device is disabled or lost. All group members are responsible for knowing and securely storing password information for various means of storage. The Gruebele group has never had a complete data loss because back-ups were always available. A complete loss, except for some small amount (a day's worth) of recent data not yet backed up constitutes unacceptable negligence and can result in changes in the assigned project or increased supervision of data integrity.

Publication preparation

- All publications with Martin as last author must be prepared using a recent version of Microsoft Word, Microsoft Equations for typesetting equations, and Zotero to manage the bibliography. This is for current and backwards compatibility. Group members may use their preferred plotting and image software, but 300 dpi LZW-compressed TIFF files for image panels and PowerPoint for vector graphics are preferred. When importing components of a figure into PowerPoint from another package, consider doing as much panel labeling and line art within PowerPoint, and as little as possible within

the imported TIFF files. Group members may use publisher's Word templates if available. For collaborative projects with other groups, different software may be used if someone else submits the paper.

Group equipment and responsibilities

- Group jobs are assigned once a year at the first fall group meeting, along with group-specific safety training. In addition, all group members are encouraged to participate in a semesterly lab cleanup to keep things safe and tidy. Martin can be consulted if an old or unknown supply or equipment is found that may be 'tossable.'

5. Interpersonal relationships

Expectation of conduct

- All group members are expected to uphold the highest level of ethical conduct. We follow the policies of the University of Illinois regarding conduct such as fabrication of scientific results. Martin and the Department Head are good contacts if you have concerns.
- All group members are expected to maintain an environment free from harassment and discrimination for all, regardless of race, gender, sexual orientation, disability, physical appearance, religion, and other identifiers, 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 Martin or to the Assistant Director of Graduate Diversity & Program Climate immediately, or to both.
- Behaviors such as unwelcome sexual attention, inappropriate touching, intimidation, or any other behaviors which contribute to a hostile workplace environment are unacceptable. If you have concerns, please consider reporting them to Martin or to the Graduate Diversity & Program Climate Director immediately, or to both. As a mandated reporter, Martin is required to report any sexual harassment or abuse he becomes aware of to the Title XI coordinator. The Graduate Diversity & Program Climate Director can provide information on who to report to confidentially.

Conflict resolution

- Interpersonal conflicts between group members are best brought to Martin's attention by all parties involved asking for a meeting via email (for the record) that Martin will mediate. It is Martin's job to listen carefully and provide advice, or refer group members to a higher level of mediation. Such conflicts can take many guises, ranging from authorship (see p. 1 and 2), to scheduling lab time or instruments, to problems of group members collaborating on a project or in a mentoring relationship. It is important for the parties involved to have a conversation first before escalating to the PI or department.
- If the conflict is with the PI, the Graduate Diversity & Program Climate Director and/or Department Head should be consulted, or the student affairs dean at the Graduate College if the group member prefers a more at-arms-length confidant.
- There is no reporting hierarchy in the group, and all members are encouraged to meet with Martin for advice, feedback, progress reports, concerns, or any matters that arise. Mentees are strongly encouraged to listen to their mentor's advice (e.g. undergrad-grad or grad-postdoc or beginning grad-senior grad) first, and these relationships do not require Martin's constant presence or intervention, unless a conflict arises.

Mental health

- Martin is always available for students to discuss mental health issues and encourages such inquiries. He understands that students may wish to consult with Mental Health professionals instead or first, and the Chemistry Department website provides a detailed list of available options. All such discussions will be kept in utmost confidentiality.

6. Lab safety

- Group members are expected to maintain safe laboratory practices at all times, including the use of appropriate PPE when in laboratory spaces. As a PI, it is Martin's responsibility to ensure students are maintaining safe work practices, and he will provide annual training and enforce this appropriately.

- Students must receive proper training (SCS Safety Checklist, all researcher-specific DRS training, the Gruebele group-specific training to be signed off on) before any experiments can be conducted in lab. For more information about safety, refer to the lab safety officers, appropriate safety documents, or the following resources:
 - o For more information, see UIUC Chemistry Joint Safety Team at <https://publish.illinois.edu/chemistryjointsafetyteam/> and Division of Research Safety: (DRS) at www.drs.illinois.edu.

7. Amendment of the group manual

- The manual must be discussed annually at a group meeting, so updates or new sections can be proposed. The first fall safety meeting is the default. Group members (that includes Martin) may bring up proposals for change at any time during the year. Any proposed changes must be discussed at a group meeting before Martin makes the decision whether they are to be incorporated in the manual.

8. Bibliography and links

Useful text on managing labs: C. Cohen, S. Cohen, “Lab Dynamics: Management and Leadership Skills for Scientists,” ISBN-13: 978-1936113781

Mentoring and professional development, Grad College: <https://grad.illinois.edu/mentoring>

Ombudsperson and problem-solving, Grad College: <https://grad.illinois.edu/ombuds/problem-solving>

Thesis support, Graduate College: <https://grad.illinois.edu/thesis>

Action Plan for Climate and Diversity, Chemistry: <https://chemistry.illinois.edu/climate/climate-and-diversity-action-plan>

Mental Health resources, Chemistry: <https://chemistry.illinois.edu/climate/mental-health-resources>

Ombudsperson and problem-solving appointment, Chemistry: See link to Dr. Munjanja at <https://chemistry.illinois.edu/diversity>

Reporting of incivility, Chemistry: <https://chemistry.illinois.edu/climate/notify-department-incivility>