



Maintaining a high degree of research productivity at a predominately undergraduate institution as your career advances

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Abstract

In this perspective, two experienced academic administrators who are computational chemists discuss strategies for how to maintain an active research program at a predominately undergraduate institution as your career progresses. More responsibility equates to less time for research, so planning for research to remain a priority is essential. We all have the same amount of time, so figuring out how to use yours better is the key to remaining active. Professional organizations such as Council on Undergraduate Research, consortia of computational chemists such as Molecular Education and Research Consortium in computational chemistry and Midwest Undergraduate Computational Chemistry Consortium, and attendance at professional conferences can help sustain your research program. Collaborations with faculty at other institutions provide a particularly effective accountability mechanism as well. Perhaps the best way to improve your productivity is to become a better mentor to your undergraduate students. Building a research group that is fun and exciting develops a culture that sustains itself and provides the momentum necessary to maintain progress toward scientific goals.

KEYWORDS

career advancement, computational chemists, research productivity, scholarly excellence

1 | INTRODUCTION

Faculty at all institution types face growing time pressures as their careers progress that can conflict with their desire to maintain a high degree of research productivity. Associate professors and professors face more calls for service, including formal administrative roles that require much time and energy. Faculty who work at predominately undergraduate institutions (PUIs) face added factors: that they teach many classes during the academic year and that their research students are undergraduates. Computational chemists at PUIs also tend to work with many students who have not yet had physical chemistry, computer science, or related advanced coursework that is standard for graduate students. In this paper, two computational chemists at PUIs who have maintained active research programs over multiple decades as their own careers have progressed provide some suggestions for how to keep publishing despite the distractions that come with progression through the ranks of the academy.

2 | BACKGROUND OF AUTHORS

George Shields has been working with undergraduates on research projects since his graduate school days at Georgia Tech and his postdoctoral time at Yale University. His own independent career started in 1989 at Lake Forest College (LFC), and he moved to Hamilton College (HC) in

1998. He chaired the LFC and HC chemistry departments for a total of 10 years before he was appointed as the founding dean of the college of science and technology at Armstrong Atlantic State University. At Armstrong, he created the first summer research program and set up a system for supporting undergraduate research that survives to this day.^[1–2] After Armstrong, he served as the dean of the college of arts and sciences at Bucknell University for 6 years, followed by a 3-year appointment as Vice President for Academic Affairs and Provost at Furman University. His 11 years of Dean/Provost experience ended in 2019. He has a wide variety of research interests and has worked with 124 undergraduate research students to date, with 90% of his alumni pursuing further education, including 40% who entered Ph.D. programs. To support his undergraduate research program, he has received more than \$6.0 million in external research and educational grant support for 31 proposals funded by NSF, NIH, ACS/PRF, Dreyfus Foundation, Research Corporation, and other funding agencies. He has published 92 scientific research papers, including 60 papers with 62 undergraduates working in his research group since 1991. According to the Web of Science database, his work has been cited more than 5000 times by other researchers, and his h-index is 35.

Scott Feller was introduced to research as an undergraduate at Willamette University where he and his mentor examined single-ion thermodynamics and published a pair of papers in the *Journal of the Electrochemical Society*. After earning a PhD in statistical mechanics with Don McQuarrie, he chose a postdoctoral position at the NIH focused on molecular simulation in order to develop a research program more suitable for working with undergraduate collaborators. He began a tenure track appointment at Wabash College in 1998 and was awarded an National Science Foundation's Research at Undergraduate Institutions (NSF RUI) grant by the Molecular Biophysics cluster, a grant that has been continuously renewed for over 20 years. Following tenure, he was named Chair of the Department of Chemistry. He was subsequently chosen as Chair of the Division of Natural Sciences and Mathematics, a role that included shared responsibility for hiring and tenure and promotion reviews. In 2014, he was named Dean of the College, Wabash's chief academic officer, and was recently appointed Acting President of the college. In addition to teaching, research, and service to his institution, he has provided leadership to the Council on Undergraduate Research (CUR) and has served as an editorial board member of multiple journals and as a regular review panel member for NSF and NIH. He has published 76 peer-reviewed papers, and according to the Web of Science database, his work has been cited more than 9000 times by other researchers, and his h-index is 38.

3 | ADVICE AFTER TENURE

3.1 | Staying focused

The road to tenure at a PUI typically requires the demonstration of excellence in teaching and research. After tenure, a newly minted Associate Professor often experiences an expectation to pick up more service assignments, both within the department and across the college or university. After working so hard toward the goal of tenure, it is not unusual for new associates to feel at a bit of a loss. Those who do not make plans for the next goal, such as achieving full Professor status, are at risk of not progressing in their careers. Various administrative roles become available, and these too risk hampering research productivity, particularly research with undergraduates. You can, however, balance these conflicting demands. The key is planning your research agenda to avoid a potential post-tenure stall. One very positive way to think about tenure is that it gives you complete freedom to explore new research areas. The best way to stay motivated is to work on projects that you are passionate about.

3.2 | The nature of our research

Computational chemists have an advantage when it comes to working with undergraduates, in that when students get busy and take a break from research during the academic year, it does not necessarily lead to immediate disaster. Abandoning a protein preparation or an organic synthesis halfway through the process ruins the experiment, but simulation results will sit safely on a computer server until students have time to examine them. Computational chemistry is also safer than wet lab chemistry, and students can work on their own from anywhere as long as they have a computer available. The biggest problem in working with students is best described by the old saying about computers: garbage in, garbage out. Despite your best efforts, your students will learn by doing, which means running many jobs that will not generate useful data as they learn the initial bewildering processes that are unique to every lab. This makes it critical to check long jobs prior to submission so that the queue is not saturated with what will eventually be junk results, with the side effect of much wasted computer time. Each failure, of course, is a chance for students to build up their knowledge base and become better at thinking through what they are trying to accomplish.

3.3 | Finding time

There really is less time available after being promoted to Associate Professor.^[3] The most common difficulty is that, while your institution has all sorts of expectations for you that have hard deadlines, most research deadlines are internally imposed. So, one way to combat this is to use your

calendar to block out time for your priorities. If your schedule is blocked on Thursday afternoon from 2 to 4 PM for a group meeting, you cannot accept another meeting request from the Parking Committee (!) or another group unless it is a true emergency. Putting proposal deadlines on your calendar, with reminders at strategic points in the process, will help you work on that big project. We have always advised our faculty to do at least one thing every day that advances your own research agenda. An effective strategy for protecting research time is the creation of accountability mechanisms so that research tasks are as important as those related to service and teaching. An example is setting a deadline that you share with a writing group or with your research collaborators.^[3]

Service opportunities requested from senior administrators can be particularly stressful, and it is helpful to talk with your departmental chair or other senior person to help you decide when to accept and when to gracefully say “thank you, but not this time.” Female faculty and faculty of color can be particularly overtaxed, especially if they are scientists, so figuring out a strategy to protect your time is very valuable. As longstanding deans, we feel that if you explain what you are trying to do to your own deans, and why you do not have time to serve on committee X because you are trying to finish project Y, which is absolutely essential for you to be promoted to Professor, that they will accept your reasons and ask someone else. And if they do not, then remember, you have tenure.

Email is a particular problem. It is always on, and people are always using it to ask you to spend time responding. You can, however, turn off your email for large portions of the day and only turn it on when your mind is too tired to focus on teaching or research anymore that day. One idea is to check it first thing in the morning and only answer the critical emails, then turn it off until the end of the day, and go through all of them in the last hour of your day. Another is to use the option in your email client to send out your email replies at a later time so that you do not end up in email dialog where your response immediately generates another. Whatever your strategy, it is important to have one because the email volume can become crushing as you move up the administrator ladder. It is crucial that you have an email strategy.^[4]

3.4 | Use the resources from the CUR

The CUR was founded in 1978 by Brian Andreen, a program officer at Research Corporation, and 10 chemistry faculty at private PUIs. At its founding, CUR was dedicated to proposing funding mechanisms to support undergraduate research at PUIs, and the efforts of the founders led to the NSF RUI program in 1983. CUR eventually expanded to all disciplines and currently serves as the preeminent organization dedicated to supporting faculty who are working with undergraduates on research projects. Many colleges and universities have become institutional members of CUR, so their entire faculty is eligible to join CUR at no individual cost, and the institutional fees are just a few thousands of dollars per year. CUR has a host of resources available on its website, and members of CUR have critical support for their undergraduate research activities.^[5] A compendium of specific examples of research-supportive practices in the curriculum is quite thought-provoking.^[6] CUR has published an edited book, *Characteristics of Excellence in Undergraduate Research (COEUR)*, which it uses as the basis of its training workshops and for its Campus-Wide Award for Undergraduate Research Accomplishments.^[7] This excellent resource contains 12 COEUR along with a template to use for self-rating of your own institution.^[8] Each characteristic is fleshed out in full in this chapter,^[8] and the rubric can be downloaded from the CUR website. Briefly, the 12 are Campus missions and culture, Administrative support, Research infrastructure, Professional development opportunities, Recognition, External funding, Dissemination, Student-centered issues, Curriculum, Summer research program, Assessment activities, and Strategic Planning.

Undergraduate research is the highest of the so-called high-impact practices because the nature of working on an original research project that is mentored by a skilled professor is absolutely transformational. Kerry Karukstis served as CUR's president during the 2007 to 2008 academic year and has written a history and analysis of the undergraduate research movement.^[9] Likewise, Crowe and Brakke have recently published an annotative bibliography on the assessment of undergraduate research.^[10]

3.5 | Becoming a better mentor

Undergraduate research is the ultimate exemplar of all of the so-called high-impact practices, but it requires careful mentoring. Mentors are vital for ensuring the success of the student experience.^[11] Faculty who work at PUIs are driven by both research and teaching, and so, seeking to become a better mentor to your students and colleagues is always a great use of time. In addition, time spent becoming a better mentor will increase your research productivity. It also tends to make the job more fun. Mentoring is essential to an authentic undergraduate research experience. This is so important that faculty should really plan how they will mentor their students before or as they recruit them. Some ways to better mentor students who are working on undergraduate research have been described in the CUR Chemistry Blog and start with how we recruit students, how they are supervised, and how the students' time in the project is ended.^[12] Check out other mentoring resources on CUR's website.^[5]

3.5.1 | Recruiting students early

One tactic for staying as productive as possible is to run a research group that is similar to a graduate school group. In graduate school, the senior researchers mentor the newer graduate students so that new students learn what they need to be productive. This clearly helps the productivity of the lab and is essential for continuity. PUI faculty, however, do not have the luxury of working with full-time researchers all year long, for four or so years. At PUIs, the bulk of concentrated research takes place in an intensive 10-week summer session, which then allows the most motivated students to continue doing some research during the academic years while maintaining a heavy course schedule. Some PUIs have funds available to pay student researchers during the academic year as well. Students are very busy, and if every computational or physical chemist waited until their undergraduates had all the coursework they needed to be “ready” to do research, then very few students would pursue research during their undergraduate days. However, if you set up your research group so that you have experienced juniors and seniors who can help you teach the first-year and second-year students who are new to the group, then you will greatly decrease your workload while increasing your productivity. This also tends to increase the satisfaction that students have with their research projects as teaching someone else what you already know increases self-confidence. Undergraduates may be less prepared for independent work, but they make up in enthusiasm what they lack in knowledge, and they often can be taught quickly. Students respond to your enthusiasm, so talk about your scholarly interests in your classes and encourage interested students to meet with you. Keep in mind that students underrepresented in STEM fields may not have the confidence to seek you out, but you can call them and offer them a place in your lab. Shields has recruited many students (female and underrepresented), as well as future Goldwater Scholars, with the simple technique of reaching out to excellent, but shy, first-year students. When you talk with prospective researchers, tell them the success stories of your prior students, such as those who have published with you or proceeded on to greater things. Make use of university and departmental resources to attract interested students, for example, university databases and/or departmental billboard space. Finally, you can ask undergraduate or graduate teaching assistants to recommend undergrads in your area and encourage your current students to recruit their own replacements.^[12]

An edited book has been published on the benefits of introducing undergraduates to research as soon as possible, and here, we reproduce the forward that Shields wrote for *The Power and Promise of Early Research*^[13]:

The difficulty of undergraduate research is scale. To be truly authentic, and thus transformative, emerging scholars in the lab need to be guided by experts who clearly care for their junior collaborators. This apprenticeship model is time consuming, absolutely essential, and difficult to scale. This is why predominately undergraduate institutions (PUIs) have led the way in guiding generation after generation of undergraduates through authentic research experiences. It is why PUIs send a higher percentage of their graduates on to graduate school than do our large research universities. To provide more undergraduates authentic research experiences to students, dedicated teachers have developed the idea of course-based undergraduate research experiences (CUREs), so that more students can be exposed to undergraduate research. This book is replete with successful examples of CUREs.

In this ACS Symposium book, Desmond Murray has organized a compelling narrative, starting with a comprehensive overview of how authentic, early research is a strategy for student success. This book shows the importance of early introduction to authentic research for all students, including those that are most likely to be left out during the normal sink or swim research university science curriculum. I can vouch for the importance of research in high school leading to real science, as many of the most important contributions my own group has made to science stem from a high school or first year college student project. After a series of interesting chapters on early research and interesting CUREs, the book's penultimate chapter is a fascinating description of student experiences, told in the impacted students own words. All of us who have worked with students on undergraduate research projects know the truth of these statements, and our mission should be to ensure that more students are exposed to the power of authentic, early, high school and undergraduate research experiences.

At Hamilton College, early introduction to the research model reinvigorated the department, resulting in outcomes such as increased number of majors, amount of money raised to support research, faculty scholarship, faculty development, and overall resources available to the department.^[14] Students were recruited to start summer research the summer before they enrolled at Hamilton and continued their research in subsequent years and summers.^[15] A statistical analysis of selected students vs a control group of applicants showed that a significantly ($P < .05$) higher percentage of program participants (76%) selected a science or math major than nonparticipants (55%). In addition, participants had an overall increase in their Hamilton grade point averages of 2.5 percentage points out of 100 after controlling for all other variables. The retention rate for participants was 98%, while the retention rate for the control group was 88%. In addition, early introduction to research improved recruiting of high school seniors, and surveys showed that the very existence of the program was influential in their selecting Hamilton for their college career.^[15]

Early introduction to research works everywhere. A stunning example was at Armstrong, a cash-poor regional PUI that had not been able to start up a summer program prior to Shields arriving as dean. He was able to cut through the red tape and set up a summer research program that included the same early introduction to research program modeled after Hamilton, but with more emphasis placed on math skills and mentoring

throughout the program.^[1-2] Despite a less strong high school preparation background for Armstrong students, as a consequence of under-resourced Savannah public high schools, this program increased retention and graduation rates significantly. The average 4-year graduation rate for first-time first-year students at Armstrong during the grant period was 6.1% for STEM majors and 13.2% for all majors. For the cohorts in the early research program, the 4-year graduation rates averaged over 40%.^[2]

One caveat of the early introduction to research model deserves mentioning. Remember that each student is a unique individual with initial goals when they start college, which are subject to change over time. It is important to understand the motivation of your students and do your best to work with those who will benefit the most from starting in the earliest stages. Some students will want to switch to experimental work after a year or two of computation, and others will want to take advantage of internships or other opportunities that the college environment provide. A great mentor supports their students as their goals change and helps them along to their future success.

3.5.2 | Supervision

Mentoring an undergraduate is an investment in the person, not just the researcher. You should connect regularly, at least weekly, with your mentee. These connections could be face to face, or via email, blogs, wiki... by whatever means is easiest to keep in touch with your undergraduates. Be honest about your expectations and encourage an open professional dialog with your mentee about the work. You are the model for the problem-solving and critical-thinking skills required to be successful. Requiring regular feedback in the form of lab notebooks or weekly email reports is one tested method that has helped keep students on track.

One of the ironic moments in working with students that happens all the time is when the professor walks through the lab and asks the room how things are going. The response is generally "all fine" or silence, and every single student looks as busy as can be. However, in reality, many students are struggling with what to do next, so it is important for professors to create a safe place for students to talk to you. Instead of asking them a general question and breezing back to your office, sit down and ask them to show you what they are working on and ask them if they have any questions about what they are trying to do. Remember that the process of research can overwhelm students, and they can question their own ability to make sense of what seems like chaos. Your encouraging words and frequent reference to the big picture of the research project will be well received by your students. Above all, do not underestimate the power of positive and constructive feedback.^[12]

Being new to research, many students do not understand the process of scientific research and may expect projects to proceed smoothly. Setbacks can be shocking, but they are good teaching moments on the benefits of failure. Of course, one of the great joys of doing research is when the unexpected occurs, and so, if you explain that *this result* is unexpected, and now we need to figure out why (Did we do something wrong? Did we discover something entirely new!), your students will continue to grow as scientists. Tell them not to be surprised if a project shifts focus a few times and help them learn that failure can be good. Adjusting goals along the way and discussing progress regularly will keep each research student motivated. Lab culture is also important, and creating a peer group of scholars is a good model for retaining research students. Whenever possible, encourage your research students to interact with and support each other. Research group social events can be a boon for productivity and morale.^[12]

Students who are beginners benefit from presenting their research locally or at the National Conference of Undergraduate Research (NCUR), where they will be surrounded by enthusiastic faculty and students from all over the country. We, and other colleges, have sent a large contingent of students of all disciplines to present at NCUR when the host institution was within easy driving distance of our campuses. After they develop more understanding of their work, your students are ready to present at conferences that focus more specifically on chemistry. Regional and smaller discipline-specific meetings are better for developing students than the large national ACS meetings, which are in turn good avenues for your most advanced research students.

3.5.3 | Finishing a project or your student graduates

As a project draws to a close or, more likely, a graduation date is looming, you can help your student disseminate their work by encouraging them to work on a paper or present at an ACS meeting. There are specific undergraduate sessions at all national ACS meetings: historically, the majority of undergraduates attend the spring meeting. Look for undergraduate sessions in the CHED division. Students with high-caliber results are also welcome to present in the division appropriate to their projects. Be sure to look for university- and department-level funding to help offset the cost to the student.

Besides dissemination, be prepared to be a reference for professional opportunities for your student. A careful and detailed letter from a research mentor can mean an extra stipend in graduate school or securing the interview for the right job. In addition, take time to reflect on the experience of mentoring this student. Think about what worked and what did not; what will you do differently next time? Finally, some mentoring relationships can bloom into enduring friendships, and former students become new peers. Enjoy this added benefit, if it comes to you, and savor a renewed passion for your own scholarship. Seeing our students succeed in research can be as gratifying as our own scholarly achievements.

Sometimes, a particular student and a particular professor do not make a good match, and having honest conversations with your students at the end of each research period may end with a decision that some other experience might now be better for a particular student. Keep in mind that, because students who are new to research have no idea what it is like, they do not always end up liking the uncertainty that comes with any scientific project. If they understand the scientific method better as a result of the time they spent in your lab, then you can consider that a success for civilization.

3.5.4 | Assessment

Ongoing assessment is important because it can help students understand themselves better and help you become a better mentor. Shields has his students write summaries of what they have accomplished on Friday afternoon of each week of the summer research session, and their plans for the next week. This provides an opportunity for immediate correction and feedback. Having your students fill out a survey at the beginning and the end of the summer session is also an excellent way for your students to reflect on what they have learned about themselves, as well as about the research project. Written reports of the students and their survey summaries make writing that first letter of recommendation for that student much easier.

3.6 | Recruiting students of color and female students

STEM faculty who believe ability is fixed have larger racial achievement gaps and inspire less student motivation in their classes,^[16] which results in fewer opportunities for research experiences. Yet, early introduction to research is a best practice for all students, and it turns out that authentic research experiences, including early ones, have an even bigger impact on students underrepresented in STEM fields.^[2,17–18] Molecular Education and Research Consortium in computational chemistry (MERCURY) and Midwest Undergraduate Computational Chemistry Consortium (MU3C) faculty have experienced this first-hand, as have many faculty who have worked with CUR on expanding opportunities for undergraduate research.^[5] Progress in a highly mentored, original research project is a great confidence builder for students and brings them face to face with the real scientific method. Julie Foertsch has presented a comprehensive account of the impacts of undergraduate research programs focused on underrepresented minorities, across 15 universities, which has led to a dramatic increase in graduate school completion rates.^[17] Finally, a recent article in the *Proceedings of the National Academy of Sciences* highlights how active learning narrows the achievement gaps for underrepresented students in undergraduate STEM majors.^[18] Undergraduate research is the ultimate active learning environment, where students learn from the challenge and thrill of discovery.

3.7 | Bias in science

While it is clear that diverse groups do better science,^[19] science has a long way to go before diversity is commonplace in the STEM workforce. In fact, faculty who are underrepresented in science, which includes everyone who is not a straight, able-bodied, white male, are subject to many, sometimes subtle and sometimes not so subtle, biases.^[20–23] These have been well documented in the literature and include a preference for science faculty at research universities to hire white male students as lab managers over equally qualified female candidates.^[20] In this randomized double-blind experimental study, faculty participants rated male applicants as significantly more competent than an identical female applicant, offered the male applicants a higher starting salary, and offered more career mentoring. The female student was viewed as less competent. Both male and female faculty exhibited the same bias against the female student.^[20] Societal views of who is a scientist loom large, and May Berenbaum has discussed the history of science in American by focusing on the most elite group of scientists, members of the National Academy of Sciences. The National Academy actually had a lower percentage of female members than Congress in 2019, 16% for the Academy vs 20% for Congress.^[21] There are fewer women and faculty of color at higher academic ranks across almost all academic institutions.

Quantitative tools have been developed to measure women's perceptions of subtle gender biases within academia, and these have been used to reveal that Associate and full Professors perceive more inequality and biases relative to Assistant Professors.^[22] Black or African-American applicants are 10 percentage points less likely than whites to be awarded NIH research funding after controlling for the applicant's educational background, country of origin, training, previous research awards, publication record, and employer characteristics.^[23] Kathleen Grogan has documented that women scientists receive less funding, publish less, are cited less, and have less recognition and visibility.^[23] These documented problems for anyone who is "other" cannot be solved without the entire STEM community working to confront this problem. Fortunately, bias can be countered by calling it out and paying attention to it and using the data to convince our coworkers that bias problems are real and can be addressed.^[23] For faculty of color and female faculty, finding allies who understand implicit and explicit bias and actively work to counter it is incredibly helpful. Likewise, PUI faculty in general, regardless of their race or gender, oftentimes feel the bias from faculty at research universities,

who sometimes make it clear that anyone working at a PUI must not be a real, committed scientist and is therefore less deserving of being supported.^[24]

A recent study from a multi-institutional research collaboration assessed the role of perceived support and local culture in how underrepresented minority faculty members mentored undergraduate research students.^[25] The authors discovered that departmental and institutional support were the key factors correlated with excellent outcomes in mentoring undergraduate researchers and that this support was more important for faculty of color than for white faculty. Their results provide evidence for the importance of institutional policy to facilitate underrepresented faculty participation in the practice of mentoring undergraduate researchers.^[25]

3.8 | Finding allies

Working at a PUI as a computational chemist often means you are teaching five to seven courses a year, including the physical chemistry courses. At many PUIs, only one faculty member is the physical chemist. As a consequence, it is very useful to meet fellow computational chemists at other PUIs who can share tips on how to manage a high teaching load with a productive undergraduate research program. The two largest organizations that support computational chemists at PUIs are the MERCURY^[26] and the MU3C.

MERCURY, founded by Shields in 2000, has grown to 38 faculty at 33 institutions. Supported by six NSF-Major Research Instrumentation (MRI) grants since 2001,^[27] MERCURY is known for scientific excellence, the diversity of its faculty and students, and for its outstanding summer conferences.^[28–29] Faculty in MERCURY have a peer review publication rate of 1.7 papers/faculty/year, which is 3.4 times the average rate for physical and natural science faculty at PUIs.^[30] Since 2001, over 1000 undergraduates have worked with MERCURY faculty, and approximately 75% are from groups underrepresented in chemistry. Approximately half of all alumni have pursued advanced degrees in STEM fields, and two-thirds of this group have been female and/or students of color. The MERCURY conferences, held at the end of the summer research season, are open to all faculty and students and have an atmosphere that feels like a Gordon Conference just for undergraduates and PUI faculty. More than 1600 participants have attended the 18 MERCURY conferences, and 61 of the 111 speakers were scientists of color and/or female.^[28–29] Many of the participants at MERCURY are faculty and students who are not members of MERCURY but benefit greatly from the networking and the exposure their students obtain from the other conference participants. Any undergraduate or faculty member can participate in the MERCURY conferences.^[26]

The MU3C is the second successful model of computational chemists at PUIs coming together to share computational resources; to provide opportunities for students to present their work; and to create a community of teacher-scholars that exchange best practices on teaching, mentoring, and research. Like MERCURY, an important component is an annual summer conference that brings together the participating research groups. The MU3C model is to recruit computational chemists at R1 universities to host the group at a different Midwestern university each year, allowing the MU3C faculty and students to interact with R1 faculty and graduate students and expose the undergraduates to potential PhD mentors. MU3C holds a second virtual conference each winter where students present posters of their work online over several days, and a discussion board mechanism is used for all participants to submit questions and comments.

3.9 | Conferences and collaborations

You can forge collaborations with experimentalists who work in areas that are exciting to you and bring your knowledge and expertise to the collaboration. Collaborating with colleagues at research-intensive (R1) institutions is a growing trend for researchers at PUIs. Because such partnerships are being initiated at a remarkable pace, Rovnyak and Shields published a book chapter that discusses emerging norms and best practices that can help these two very different research cultures build successful and lasting relationships. This article describes a chronological roadmap for all stages of a PUI/R1 collaboration, with emphasis placed on strong communication between partners. A focus on elucidating mutual expectations and leveraging the respective strengths of the PUI and R1 partners is essential for success.^[24]

One of the best ways to form collaborations and get good advice stems from meeting people at conferences, and a good strategy is to use the limited travel funds available at most PUIs to attend smaller, more disciplinary-focused meetings, where you have the best chance of meeting PUI and R1 faculty who share your research interests. Smaller meetings make it easier to meet people, which is of critical importance. As most conferences do not separate the undergraduate posters into a separate category (and if they do, like ACS national meetings, you can choose to submit to the COMP, PHYS, or other sessions instead), not only are your students getting great practice defending their science, but it also increases the opportunities to meet scientists with shared interests and complementary expertise. Oftentimes, the posters that your undergraduates present at meetings bring together scientists who are quite interested in your work. Beyond collaborations, a meeting of the minds around a poster presentation often leads to great advice or future directions of a project. The success of an RUI project often depends on the advice received at one of these poster sessions!^[24] Of course, computational chemists should strongly consider sending their undergraduates to the MERCURY conference, which is held near the end of the summer research session and, like a Gordon conference, is focused on undergraduates

and PUI faculty.^[29] Much PUI faculty success stems from interactions between the research faculty who are the invited speakers and all the PUI faculty in attendance, with undergraduates as the vital connecting force between them.^[28]

3.10 | Finding resources

We like to say that you can never have enough money to support your research program, a message driven by the high cost of doing science and the flexibility that funding provides. Faculty have many great ideas, and supporting faculty as they write proposals is an essential activity. PUI faculty have a variety of funding resources, and they need to make use of them, so they can support their own research program, including computers, software, and student and faculty summer salaries. A competent grants office that can help eliminate the bureaucracy of proposal writing, as well as a backend function to keep track of how the money is being spent, is a godsend. Important funding resources for PUI faculty at this time are the Petroleum Research Fund managed by the American Chemical Society (ACS/PRF), Research Corporation for Science Advancement (RSCA), NSF, NIH, Department of Energy (DOE), Department of Defense (DOD), and the Camille and Henry Dreyfus Foundation.

ACS/PRF provides funding for research that is petroleum related, and an inquiry to the program officer will help you decide if your research can fit into their portfolio of what they consider petroleum related. RSCA has a competitive program for Cottrell Scholars, requiring a research and education proposal, and is available only to faculty at the end of their third year in a tenure-track faculty position. Cottrell Scholars come from both PUI and research institutions, and they have continuing opportunities for funding from RSCA throughout their careers.

NSF has a special program for PUI faculty, known as the RUI program. The purpose of the RUI program is to support PUI faculty in research, build research capacity at their home institutions, and support the integration of research and undergraduate education. Eligible PUIs are accredited colleges and universities, including 2-year community colleges, that have awarded 20 or fewer Ph.D./D.Sci. degrees in all NSF-supported fields during the combined previous 2 years. Any research proposal to an NSF program from a PUI is reviewed with all other proposals, but a RUI proposal has an additional (five-page maximum) RUI Impact Statement that allows faculty to make the case for how this award would enhance research activities at their institution. RUI proposals may request support for an individual or collaborative research project involving PUI faculty at their own or other institutions or may request shared instrumentation. The Chemistry division of NSF currently provides awards in the eight disciplinary areas of Chemical Catalysis; Chemistry of Life Processes; Chemical Measurements and Imaging; Chemical Structure, Dynamics, and Mechanisms (A and B); Chemical Theory, Models, and Computational Methods; Environmental Chemical Sciences; Macromolecular, Supramolecular, and Nanochemistry; and Chemical Synthesis. In addition, NSF Chemistry has four integrative programs in Centers for Chemical Innovation, MRI, Research Experiences for Undergraduates, and Special Projects and Initiatives. Chemistry sits within the Directorate for Mathematical and Physical Sciences (MPS). Other divisions in MPS that have funding that may be applicable to some chemists are Astronomical Sciences, Materials Research, Mathematical Sciences, and Physics. Other directorates at NSF that chemists could apply to for funding include Biological Sciences, Computer and Information Sciences, Education and Human Resources, Engineering, Environmental Research and Education, Geosciences, Integrative Activities, International Science and Engineering, and Social, Behavioral and Economic Sciences. NSF also has 10 Big Ideas they are interested in funding, many of which will be of interest to computational chemists.

NSF proposals are reviewed for intellectual merit and broader impacts. We suggest you write to program officers or schedule a phone call to talk about your research idea to find out if it fits in their portfolio before you apply. Currently, most chemistry division proposals are accepted in September or October, depending on the program. Proposal pressure from PUI faculty for research funding is not as high as you might imagine, so a good proposal has an excellent chance of being funded. In addition, if you are not funded, if you take the reviewer comments to heart and rewrite and resubmit, you have a good chance of being funded in the next cycle. Funding rates for research proposals at NSF hover around 30%. All awards are searchable on the NSF website, and anyone serious about supporting their undergraduate research program will be well-served by exploring funding options and developing a funding strategy. There are two important things to keep in mind: First, faculty who do not resubmit after the first submission is turned down are committing a fatal flaw because you cannot get money for research if you give up after the first submission is turned down! Second, you must publish your research to increase your chances of being funded. Unpublished research findings do not exist in the literature!

The MRI program at NSF serves to increase access to multiuser scientific and engineering instrumentation for research and research training. These awards support the acquisition or development of multiuser research instrumentation that is too costly to support through other NSF programs. The MRI program has funding rates approaching 50% and is a valuable source of equipment funding at PUIs for instruments that serve a dual role for education and research.

Another funding option at NSF is a Research Opportunity Award (ROA). An ROA is a supplement to an existing NSF award to support ROA activities for PUI faculty, or it can be a submission of a new collaborative proposal between a PUI and another institution, with an ROA component as a subaward or as part of a linked collaborative proposal. The Faculty Early Career Development Program (CAREER) awards are also available to PUI faculty. Applicants to the highly competitive CAREER award must be Assistant Professors and can submit up to three times in the competition. RUI impact statements are not allowed in CAREER proposals.

NIH has a similar program to RUI, known as a Research Enhancement Award (AREA, or R15). This award currently funds a PUI faculty member for 3 years with a total direct cost limit of \$300 000 and is renewable. AREA awards currently have three submission dates, and the same caveat applies about publishing your research to retain funding for subsequent research. Other agencies where PUI faculty have had success in obtaining funding include the DOE and the DOD. Interestingly, DOD has funding to support a variety of diseases that veterans suffer from, including most cancers.

The Camille and Henry Dreyfus Foundation is dedicated to the advancement of the chemical sciences. The Henry Dreyfus Teacher-Scholar Awards provide a \$75 000 unrestricted research award to PUI faculty who have demonstrated leadership in original research of outstanding quality with undergraduates, as well as excellence and dedication to undergraduate education. Nominations are accepted after the 4th year of the start of an independent career, up until the 12th year. Institutions may nominate one faculty member per year, and renominations are accepted.

Some sources of money that can be applied to undergraduate research include using indirect cost overhead returns from proposals that are funded; a stipend program to faculty who are writing proposals that will pay for their research, as well as bring in more indirect costs that can support the stipend program and more research; a matching funds program to leverage proposal activity; using Work Study money to pay student stipends; working with Development to raise money for endowments and ongoing costs; and applying for NIH INBRE and NSF EPSCoR money if you are in one of the 23 states that receives the least amount of federal funding (like South Carolina). Furman has benefited tremendously from INBRE and EPSCoR money that flows to South Carolina. John Wheeler runs the office of Integrative Science and has brought in millions to Furman over the past 15 years to support the work of STEM faculty. Hamilton College has endowed their Early Introduction to Research Program, which was originally funded by the Dreyfus Foundation, from a private gift from a parent (who's son was in the program and then went to MIT for graduate school). Many other PUIs have similar endowments to support undergraduate research opportunities. The John Stauffer Charitable Trust has helped PUIs in California establish endowments for summer research in chemistry. As a highly mentored undergraduate research experience is the best example of a transformative high-impact practice, many colleges have included raising endowments to support undergraduate research in their capital campaigns.

3.11 | Professors

Once you have achieved the rank of Professor, you have shown that you can balance your teaching, research, and service responsibilities. At this point, you have many options, which include leading the department, helping to build a department that is focused on high-impact undergraduate research opportunities,^[14] mentoring junior colleagues, and leading by example. The best PUIs for undergraduate research are continually building up their resource base, providing more support to bring this high-impact practice to as many students as possible. Undergraduate research offices, grants offices, grants accounting, development staff to raise funds, divisional staff to support instrumentation and repair, and clerical support to handle paperwork are all ways that PUIs support the undergraduate research enterprise. Many professors have been essential in maintaining and improving the research experiences on their campuses. Hanover Research has published a comprehensive report on the essential characteristics of institutions with high levels of research productivity and, although written with research universities in mind, has some ideas that might be useful at PUIs.^[31]

4 | ADMINISTRATIVE RESPONSIBILITIES

In an ideal world, only full Professors would be thrust into administrative roles, but of course, we live in the real world, and often, institutions, and faculty themselves, do not want to wait that long before they take on more university-level service. Indeed, Shields became Chair of the department at Lake Forest 1 year after being tenured and promoted to Associate Professor. Colleges and universities have all kinds of administrative roles that are part-time, ranging from running the undergraduate research program, to associate dean and associate provost roles with specific responsibilities, to chairing a department. What all of these have in common is that they generally rely on course releases or a stipend for compensation. These roles should have term limits and a clear mandate, so you know when you are doing your administrative role, when you are teaching, and when you have time for research. Good Deans and Provosts will support your research program. When negotiating these roles, be cautious about how much time you are committing to teaching during your first year as you will need time to learn your new role while keeping your research program afloat.

A great way to prepare for administrative responsibilities is to find an appropriate workshop or two that will help you think about some of the issues you will confront and figure out if this is something you want to try. One excellent resource is the Academic Leadership Training workshop run by Rigoberto Hernandez at Johns Hopkins University, hosted by ACS and sponsored by ACS and Research Corporation. The 2.5-day workshop for researchers in the field of chemistry, physics, or astrophysics helps train the next generation of academic leaders by providing them with the tools, connections, and skills to be successful as a research center director, department chair, college dean, or provost.^[32] Generally, half

of the 35 to 40 attendees are from PUIs. An excellent way to begin a stint as an administrator is with a clear idea that you will return to the faculty after your term, so maintaining your scholarship is an essential activity during your administrative role.

4.1 | Department chairs

Most department chairs at PUIs are not full-time jobs but come with a course release and/or a small stipend. The compensation rarely makes up for the actual loss of time that you have to spend on departmental responsibilities. It is our feeling that if you take on this job, then you should do it because you want to lead your department, which means taking the hiring and mentoring of your colleagues very seriously and leading a strategic planning process with a goal of improving the education provided to students. When Shields arrived at Hamilton College, weekly meetings to discuss issues and a retreat at the end of his first year led to a strategic planning process whereby the faculty together were able to greatly improve undergraduate education. By focusing on teaching smaller class sizes in the first 2 years of the curriculum, and with the goal of providing as many research opportunities to students as possible, the faculty transformed the department.^[14] The department increased its number of chemistry majors from 3 to 15 a year (with another 10 biochemistry majors), increased the number of summer research students from 4 to 37, added faculty and staff, increased diversity, and raised significantly more money to support research. From 2000 to 2008, students working with chemistry faculty received 17 national awards, and 80% of chemistry and biochemistry graduates enrolled in medical, graduate, or other professional programs. Research productivity soared as the increase in the number of publications per faculty member from the decade of 1986 to 1995 to the decade of 1996 to 2005 ranked Hamilton seventh of 55 highly accomplished liberal arts colleges.^[33]

Maintaining an active research program as chair is leading by example because, if the chair can find time for research, all the faculty should be able to as well. Leading a department to make improvements while maintaining your own research productivity depends on a variety of factors of course. Some of these include learning how to delegate, managing email, holding focused meetings, and learning when you need to consult the department and when you can make executive decisions. Learning how to delegate is an essential skill if you want to maintain your research, and you should discuss this with your colleagues before you take on the chair position. To put it simply, you need their buy-in that your role as chair is to lead the conversations that will move the department forward, but the actual effort has to be shared. A good academic assistant is also important. An effective chair learns how to train the assistant to do the tasks that must be repeated over and over. Resist the urge to do them yourself because you think you can do them quicker. You will save a tremendous amount of time if your assistant handles those things that do not require a Ph.D. in chemistry! One immensely useful task is keeping a calendar that notifies you of all the usual academic deadlines that come up so that you do not miss them. Paperwork associated with majors, tracking summer research stipends from various sources, collecting data about other colleges from their websites or their departmental assistants, and keeping up the department website are all activities that an assistant can do. Brainstorm with yours to find out what activities your assistant can do in order to save your time.

Faculty tend to hate meetings because they eat up a lot of time—you can nip this in the bud immediately as chair by never meeting without an agenda, limiting the time of the meeting and not running over, and by leading a discussion of behavior in meetings so that bad behavior of the faculty is limited (no long monologues by one person, quickly returning to the subject under discussion when the conversation strays, etc.). Your HR department, Dean, or Provost will ideally give you some training on how to be an effective department chair but, failing that, will still be able to provide resources filled with ideas on how you can be efficient and effective.

4.2 | Dean/Vice President of Academic Affairs/Provost

Depending on the size of the institution, PUIs will have full-time administrators with titles such as Dean, Dean of Faculty, Vice President of Academic Affairs (VPAA), and Provost. Smaller colleges tend to have a Dean who is also the chief academic officer and so will have the additional title of VPAA and/or Provost. Larger PUIs will have deans for each college and a chief academic officer responsible for the overall academic program (VPAA/Provost). We speak from experience that the first time one holds a Dean position at a PUI feels like you are drinking from a firehose! The duties, including those other duties that pop up that were not explicitly laid out in the contract (other duties as assigned!), can be overwhelming. In order to continue to be active in research requires a good plan, much hard work, and some organizational help. Now, you will most likely have a full-time administrative assistant who can manage your calendar, your travel, and basically handle many administrative details that can quickly overwhelm a faculty member used to handling most things on his or her own. One of the most difficult parts of the job is that your time no longer seems like it is your own as everyone wants your time to pitch their idea or problem. It is very hard or impossible to find large blocks of time.

Misra and Lundquist have published an excellent column on balancing leadership with life.^[4] They provide some general strategies (Delegate; Schedule face time instead of writing long emails; Set clear expectations on when you are available; Organize your schedule; etc.) along with some practical examples. They emphasize how important it is to schedule holidays and vacations and to take them!^[4]

Staying grant active is a real boon to your program because, once you become a 12-month administrator, you can no longer pay yourself summer salary from your grant, but you can now use this money to hire people to help you mentor students. The usual idea is to hire a postdoc, but

you can also hire postbaccalaureate researchers (graduated seniors who stay for a year and finish up their research projects or want a very interesting first job) or other senior staff in the department who might like to do some research. It is also possible to negotiate for a research fund to support your work prior to accepting this position, and of course, having explicit research responsibilities written into your contract makes it easier to make time for the work. The benefits of staying research active are many, and just two of them are the respect the faculty have for continuing your scholarship and the stress-relieving break that thinking like a chemist brings to your otherwise packed day job.

Should you teach as dean? This depends a bit on the size of your college. Wabash has about 100 faculty, and as dean, Feller taught in the humanities colloquium each semester and team-taught twice. Similarly, when Shields was dean at Armstrong, which had about 70 faculty, he taught one course a year, an Honors General Chemistry course. Once he moved to Bucknell and had 300 faculty, he stopped teaching and used his limited spare time to keep his research program in motion. In general, the larger PUIs have more complicated departmental and college structures.

4.3 | Low-cost ways for deans and other administrators to support research

Sustaining undergraduate research over a faculty career is difficult, and when administrators let the faculty know how much they appreciate their efforts, this little bit of acknowledgment goes a long way. A simple written note of appreciation, some spoken words of praise and encouragement, and acknowledgment of success on the webpage or through press releases of accomplishments is often reward enough. Administrators who eliminate administrative barriers—you know, those ones the faculty constantly complain about—are doing God's work. Supporting the faculty who are the best mentors and have the best outcomes with their students stretches the resources while increasing the impact. A well-functioning Faculty Development Center or other office that teaches faculty how to be better mentors and brings the CUR resources to campus is an excellent investment. Students and faculty alike appreciate some fun activities added to the summer research program. From the Dean/Provost point of view, assessment is critical because it promotes a sustainable research program that has continuous, incremental improvement. Remember that undergraduate research is only transformative if the students are engaged in real research with an inspiring mentor, and use your limited resources accordingly.

Leadership is critical, and this is the reason why active researchers should take on academic leadership roles. As a dean you can recognize your hard-working faculty and use data to make sure your students are getting transformative experiences. Leaders have the ability to set up programs that involve students of color, low socioeconomic status, and first-generation students in transformative research projects early in their undergraduate careers.^[17–18] These students benefit the most from faculty mentoring and guidance. As dean, you can set up sustainable, meaningful assessment and continue to improve the undergraduate research program on your campus through incremental improvements. Finally, this gives you an opportunity to support your outstanding faculty who provide the best research experiences for your students.

5 | CONCLUSIONS

There is less time available to do research after reaching tenure, and essential administrative tasks of the university must be completed. You can continue to thrive as a researcher if you devote some time to planning on how you will accomplish this and use your planning to schedule the activities that are most important to you. There are plenty of resources available for how to work more efficiently so you have time for meaningful research.

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