

1. Research and the Faculty

1.1 Chemistry's Vision for the Future.

While the past century has seen incredible advances in the ability of chemists to make and break covalent molecular bonds, the current century will require similar advances in our understanding of the noncovalent forces that underlie much of biology, energy solutions, and materials science. While chemists of the past century focused on angstrom length scales (the covalent bond), chemists of the future need to be equally adept at understanding and manipulating nanometer (and larger) length scales, as in biological or material assemblies. Understanding and manipulating complex interactions, across multiple length scales, will provide exceptional control of systems critical to next generation materials, sustainability, and human health.

In keeping with the above goals for chemistry as a discipline, the Chemistry Department at UMass Amherst sits solidly at the center of interdisciplinary science. From leadership in research centers to individual collaborations, our researchers interact with faculty in most of the departments in CNS – from Biology to Polymer Science to Food Science – and within the College of Engineering. Our faculty are intimately involved in all of the centers that comprise the Institute for Applied Life Sciences, providing the strengths that solid chemical perspectives can bring to important biomedical questions.

The hiring proposal below focuses on this strategic vision, with an aim towards hiring new faculty who will complement an interactive and highly interdepartmental UMass Amherst faculty, and who will focus on unraveling the molecular basis of research problems at the interface of chemistry with biomedical and physics/materials science. We anticipate that vibrant research programs at this interface will have transformational impact in the areas of the molecular basis for disease, materials nanotechnology/surface science, catalysis, and sustainability.

As noted below, we will require about 18 new hires over the next decade to reach 34 tenure system faculty. With new space on-line and in process, we have an exceptional opportunity to repopulate Chemistry's tenure system faculty ranks and strategically position us to compete in key areas over the next several decades. We envision recruiting one out of every three hires in the next several years as mid-career or post-tenure early-career hires. This strategy will be particularly fruitful because: (a) such hires add instant credibility to our investment in an area of strength, which then makes it easier for subsequent hires of junior faculty; (b) their addition enhances the probability of succeeding in large-scale research centers; and (c) the overall return on investment in terms of reputation and funding can be much higher and faster.

Biomedical Chemistry. Massachusetts has recognized that life sciences (e.g. biomedical, biotechnology and pharmaceutical industries) are key drivers for economic growth within the Commonwealth¹. UMass plays a central role in training the life science workforce in the Commonwealth, and Chemistry contributes strongly to that effort. Since 2000, 38% of our undergraduate Chemistry majors reported jobs in the life sciences in the Commonwealth following graduation. In the past five years, 57% of Chemistry Department PhD graduates who have chosen industrial positions in the Commonwealth work in the life sciences sector.

Strategic Goal: Develop an internationally recognized team for design, synthesis, delivery, and tracking of novel therapeutic platforms. Chemists can control and interrogate biology in novel ways because of our ability to synthesize new probes, harness powerful spectroscopies, model biomolecules and biological processes, and develop new vehicles for targeted probe

¹ Barry Bluestone and Alan Clayton-Matthews. *Life Sciences Innovation as a Catalyst for Economic Development: The Role of the Massachusetts Life Sciences Center*. 2013.

and drug delivery. This interplay between chemistry and biology is where transformational and translational advances increasingly occur. The decision by the Department to invest in biological chemistry two decades ago has paid off dramatically. Although the Chemistry Department has diverse research foci, the number of NIH-funded faculty is now greater than any of our peer departments on campus (nearly 1/3 of Chemistry faculty are NIH-funded).

By building on our strengths, we have the potential to become an internationally recognized department for design, synthesis and delivery of novel therapeutic platforms. Our current strengths are in analytical and structural characterization of proteins and biomolecules and in synthesis of delivery and sensing devices. Our faculty cluster in the disease areas of cancer and neurodegeneration; we aim to augment our strength in these areas. Over the next five years we aim to make five hires to enhance our strengths and add additional capabilities. (1) To take advantage of our strength in delivery and to take advantage of the current trend toward “biologics,” the fastest growing sector of the pharmaceutical market, we aim to hire a protein engineer who will build proteins or peptides with new chemical properties. (2) To augment our analytical and structural characterization, we aim to hire an NMR spectroscopist who can correlate motions on a molecular timescale with computational analyses, to provide a detailed molecular understanding of the structural transformations in the biomolecules that we build, effect, and deliver. (3) We will also hire a medicinal chemist who focuses on making novel compounds for treating critical diseases, with a particular emphasis on cancer or neurodegeneration. (4) We seek to hire someone who develops chemical tools that allow real time tracking of proteins, RNA, polymers, delivery vehicles and small molecules within cells. (5) We have recently hired in chemical biology - the emerging field that uses chemistry to shape and probe biological processes - and also aim to expand this area with an additional hire in the chemistry of neurodegeneration. We propose that two of these hires be mid-career or senior hires with experience working with industry to translate academic discoveries to commercialization. In addition, we seek to hire two investigators with experience in relevant preclinical animal models. These hires are strategically important for our department's and campus' overall mission (we do recognize that these latter two hires could be in the Chemistry Department or in another appropriate department on campus). With these new hires, we will be well-positioned for garnering a nano-cancer program project grant from the NIH and will also position ourselves for multi-investigator projects in the areas of neurochemistry and aging.

Strategic Goal: Increase impact of UMass Chemistry technologies. Faculty in the Chemistry Department have strong ties with the pharma and biotech sector through contracts, collaborations and licensing agreements (see listing below). Building on the infrastructure of IALS and the newly organized TTO, we aim to further increase the visibility of UMass Chemistry Technologies with outside investors. We will work to establish additional industrial interactions, particularly collaborations and licensing agreements and found more companies that implement UMass Chemistry technologies. Going forward our seminar series will include two key industrial presenters each semester. In addition we will leverage ties to our expansive and engaged alumni network to advertise UMass Chemistry capabilities and technologies. For example, the Applied Analytical and Drug Design courses each bring to UMass 6-10 industry speakers every year. Similar courses with other foci will provide still more opportunities for both faculty and students to connect and establish beneficial collaborations with industry.

Materials Chemistry. While the field of materials science and engineering has been largely ‘observational and heuristic,’ chemists have focused on developing ‘predictive and quantitative’ models to develop the next generation of materials that address next generation challenges. This interface between Chemistry and materials science / physics is an area in which UMass Chemistry excels. By making strategic additional investments through hires, our vision is to create an even more emboldened, world-class materials chemistry community at UMass

Amherst that excels in the area of design and control of molecular and macromolecular assemblies at multiple length scales. We aspire for Chemistry to be recognized as a center for materials and the destination of choice for students and postdoctoral researchers interested in this area. We intend to capitalize on the existing strengths within the Chemistry Department, to build on our momentum in materials chemistry research. UMass Amherst has a strong reputation in both the synthetic chemistry and characterization techniques of macromolecular assemblies and electronic materials. Chemistry's past successes in centers such as MRSEC, CHM, and EFRC are strong indicators of our strength and momentum. Our recent results also suggest that there is a need for further investment. We will build on our strengths and identify strategic growth/goal areas with specific objectives and critical success factors. An internationally renowned and agile materials chemistry research program with core strengths that complements the existing strengths in other departments will position UMass Amherst to compete successfully for large multi-investigator grants and research centers.

Strategic Goal: Building a Core Group of Materials Chemistry Faculty. Leadership in the area of design and control of molecular and macromolecular assemblies at multiple length scales requires a core group of chemistry faculty. We envision five hires in the materials chemistry area with the following foci: (1) molecular scale self-assembly to generate novel materials. Examples include recent advances and interests in metal-organic framework materials and covalent-organic framework materials, (2) molecular scale and nanoscale characterization of ordered and amorphous assemblies, especially at the interfaces because interfaces often dictate the propagation of self-assembly in materials and are the most challenging to interrogate, (3) computation of materials characteristics to complement the existing experimental strengths within the department and the campus, (4) time-resolved spectroscopy to interrogate the chemical processes at ultra-fast time scales that are not easily analyzed under steady-state conditions, and (5) device fabrication and characterization, where analytical chemistry becomes the key driver to translate innovations in aspects of sensing and diagnostics, for example developing specific chemistries to sense analytes *in situ*. Our goal is to assemble a synergistic core group at least 14 highly interactive faculty with complementary expertise. Our objective is to add at least 6 faculty to the existing group and establishment of the core group within 4 years (we have left one position undescribed to allow for our ability to dynamic in addressing emerging areas during the time scale of our hires). Establishing this core group within 4 years is critical to our success. We will hire a faculty at the mid-career or senior level in the next two years. The areas of characterization of assemblies/interfaces or computation of materials characteristics are two especially appropriate target areas for this hire.

Strategic Goal: Building Partnerships with Industry. A successful materials chemistry program requires translating fundamental research into innovation. Partnerships with businesses provide insights into emerging frontiers, problems and constraints in translational research. Such partnerships are essential for competitiveness in large center grants and successful placement of graduate students. Our goal is to establish strong and sustaining partnerships with materials chemistry industry in the next decade.

While we have summarized two primary areas of focus in the above, there are substantial and productive synergies between the two. Again, the establishment of IALS can be a boon for this, because our fundamental innovations in materials chemistry can impact a variety of areas, including health sciences. For example, our device scientists in sensing and diagnostics would fit perfectly with CPHM and the CBD of the IALS.

Our first objective is to set up a ≈ 5 member advisory board consisting of Chemistry alumni in the materials chemistry industry, in addition to a faculty member from ISOM and a representative from UMII and/or TTO. Concurrent with establishing the advisory board, we will explore filling the expertise gaps that we need to establish major research centers.

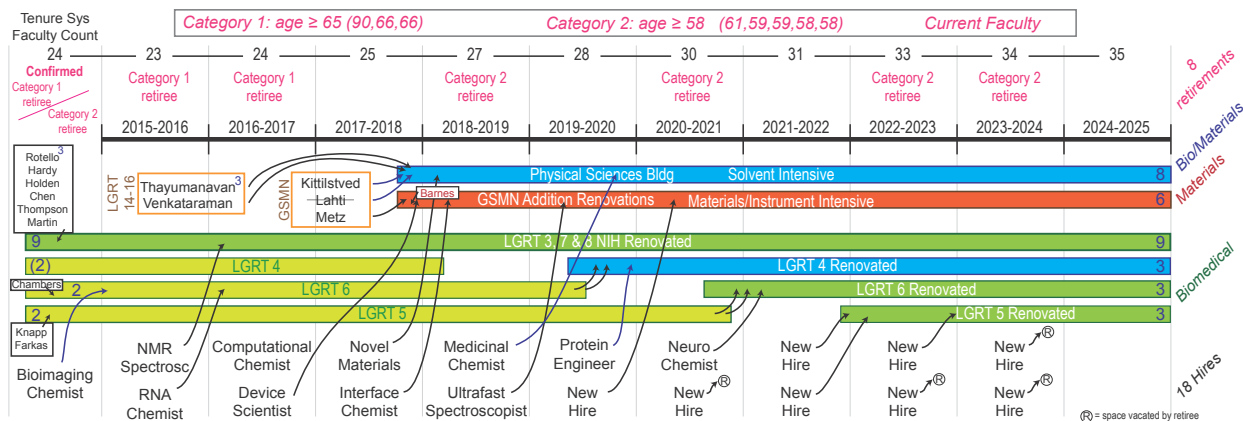
1. 2 How Chemistry will leverage existing resources

Faculty staffing. The Chemistry Department is at record low numbers of tenure system faculty and is very low compared to universities of similar size. For example, the University of Connecticut has 30 tenure system faculty and 6 lecturers, with an undergraduate enrollment of 18,000. Stony Brook University, with an undergraduate enrollment of 16,800 has 30 non-shared and 12 joint-appointment (some with Brookhaven) tenure system faculty. At UMass Amherst, in 2000, there were 30 tenure system faculty in Chemistry; today we are at 24, with *two* retiring in May, leaving us with 22 tenure system faculty as of June 2015.

While tenure system faculty dropped almost 30% during the past decade, enrollments in large service courses, taken by most majors in CNS and some in Engineering, have *increased 100%* during the same period. The University has recognized both this challenge and the investment opportunity of research in Chemistry, and has “right-sized” the department at 34 tenure system faculty. With the anticipated retirements shown below, an aggressive hiring schedule will need to commence immediately, to achieve, or even approach, the right-sized target (the timeline below requires almost a *decade* to achieve right-size numbers). Fortunately, this is an ideal time to hire new faculty in Chemistry.

Chemistry now has a record low 24 tenure system faculty (**22 as of June 2015**), down from 27 two years ago and 30 more than a decade ago (with 4 lecturers). Chemistry maintains a very large service teaching load, as the vast majority of CNS majors have 1-2 years of Chemistry lecture and lab as major requirements. During the past decade, enrollments in the sciences at UMass have doubled and continue to grow. These two factors have stretched our capacity to cover service courses, while at the same time offering state of the art advanced undergraduate and graduate level courses.

We currently employ 7½ lecturers and although they are excellent educators, we *must replenish our tenure system ranks*. An investment in tenure system Chemistry faculty is a solid investment both in demonstrated and future research excellence and in accomplished training of students across the sciences and engineering.



Staging of space, hires and retirements. Timeline showing occupancy of current and future laboratory space. Capacities before and after renovation are indicated within the bars, left and right, respectively. Three faculty (not shown) have laboratories in LSL. Two faculty (not shown) require only quality computational space. Note that all three faculty in retirement category 1 and one in category 2 either have no current space, or that space has been targeted for other units/purposes – their replacements will need to be accommodated. Two faculty, Rotello and Thayumanavan, have funded group sizes about triple that of the typical chemistry faculty; space assignments above take this into account. See Appendix for a larger version of this graphic.

Space. Current University projects present a timely opportunity to attract top talent, while addressing the challenge noted above. The Chemistry Department will be able to attract the

most competitive candidates with the promise of space in the new Physical Sciences Building (breaking ground this summer) and in to be renovated space in Goessmann labs (second floor "Goessman Addition," soon to enter design phase) that will connect directly to the PSB and to our researchers in LGRT. A substantial investment in building infrastructure improvement, completed in 2013, allows this space to be renovated to modern standards, at reasonable cost. Similarly, a funded project to replace the HVAC in LGRT will facilitate the type of renovations on floors 4, 5, and 6 that have already been completed (with the aid of federal dollars) on floors 3, 7, and 8. We are in a unique time in that swing space exists to accommodate these planned renovations (three Chemistry faculty, not shown above, have moved to LSL). Thus we anticipate only minor sprucing up of the available swing space and no significant renovations of the candidates' final space. Staging of the renovations in LGRT will largely negate the need for swing space in that phase. *This is a rare opportunity to attract the very best candidates!*

It is important to note that the new Physical Sciences Building (PSB) space represents a significant increase in quality, but not in capacity. Upon its completion, Chemistry will fully vacate floors 14, 15, and 16 of LGRT (as it recently vacated floor 13), and will fully vacate rooms 201, 202, and 142 in Goessmann. The University will repurpose *all* of this space, consistent with its capabilities. Floors 13-16 of LGRT, for example, are not rated for even minimal solvent loading under fire codes of the past two decades and will be repurposed as office space for other departments.

Similarly, the Goessmann Addition space targeted by the University for complete renovation currently reflects the lack of *any* significant renovation since its construction in the 1950s. Almost all of this space currently sits vacant, and cannot be used to recruit (or even retain) faculty. The \$9 million investment, completed in 2013, of a completely new air handling system now primes this space for renovation to "new building" standards, at reasonable costs. The decision to renovate the second floor of the Goessmann Addition to modern standards is both absolutely necessary and opportunistically timely.

Full renovation of LGRT 4, 5 & 6 will allow us to increase the number of faculty on those floors from 6 to 9 (and attract top candidates). With those new renovations and the completion of the PSB and Goessmann Addition renovations (already funded), Chemistry would not require significant new faculty renovation funds through at least 2025, and likely later. If the LGRT 4, 5 & 6 renovations begin immediately after completion of the PSB and the Goessmann Addition renovations, we would not require additional swing space to accommodate existing faculty during those renovations (and perhaps be able to renovate more than one floor at a time, saving expense).

It is essential to note that the planned Goessmann Addition renovation is intimately tied to the new Physical Sciences Building. There will be a second floor "connector" between the two buildings and space for shared instrumentation will sit at that interface, fully within Goessmann. This planning enabled the programming of maximal hood space in the final design of the Physical Sciences Building. Synthetic chemists in that space will have ready and immediate access to necessary instrumentation, immediately across the bridge. For example, synthetic chemists routinely monitor the progress of their reactions by NMR and other spectroscopies, and thus require that these tools be in close proximity. This design has a secondary and very intentional benefit as well: located between synthetic research laboratories in PSB and device/characterization laboratories in the Goessmann Addition, this space will serve as a gathering point for a large number of laboratories, fostering and encouraging existing and new interdisciplinary collaborations. This cross-fertilization, already a hallmark of science at UMass, will enable still more joint and center research grants.

1.3 Dealing with decline of federal funding

The Department of Chemistry, despite having a large teaching commitment, has been very successful in the procurement of external funding. In particular, in the face of record low numbers of faculty and serving multiple research missions, the Chemistry Department has more NIH grants than any other department on campus. That said, we clearly recognize the current tight funding environment. We have accordingly been increasing our efforts in the mentoring of junior and mid-career faculty, but we must do better. In the recent past, *ad hoc* reading of draft grant proposals by experienced faculty was common, but not well-organized. Several years ago, we initiated a monthly series of talks at which faculty (of any rank, but with priority to junior faculty) can pitch new ideas and get immediate feedback from their colleagues. We will continue this program, but also establish a more formal mechanism for the reading of and commenting on grant proposals. In the current climate, the experience gained from reviewing proposals is essential to success in crafting them.

The Department of Chemistry also has a strong history of leadership in shared and center grants. Recent examples include CCI, EFRC, MRSEC, NSEC, IGERTs, and the Chemistry-Biology Interface and Biotechnology NIH T32 training grants (see next section). Collaborations are also common both internally and externally. In fact, >80% of our faculty members have published at least one publication in the last five years with another colleague in the department. If one includes colleagues from outside the department, this number is close to 100%. Participation in such collaborative efforts provides a strength that is more than simply the sum of its parts and achieves a level of interdisciplinarity that is often essential to success in the modern era. At the same time, we will continue to expect demonstrated leadership and independence of our junior faculty, as they must demonstrate a reasonable expectation of long term success at the time of tenure.

While NIH and NSF will remain the primary sources of funding, we also have and will exploit other funding sources, specifically with respect to both materials and biomedicine: DoD and DoE. Similarly, industry support now plays and will continue to play a larger role in our research, as more efforts turn to translational outcomes. We have begun to partner strategically with IALS and the TTO to enable additional industrial collaborations and contracts. This has yielded a number of new research agreements. Chemistry faculty have been the leads in the recent startup companies Cyta Therapeutics and Protein Attachment Technologies, LLC. We recognize that industry support is typically targeted and is often shorter-term than stable federal awards. In seeking new industrial grants and contracts, we strategically select the agreements that are in our best long-term interest, so as to not jeopardize long-term federal funding.

Current industry partners

CEM Corp.
BASF
Biogen
Pepsico
Johnson & Johnson
Pfizer
Procter & Gamble
ReclaimRX LLC
Anika Therapeutics
Novartis
Photonis
Firmenich, SA
Precibio Medical Devices

1.4 Infrastructure support to achieve the vision

The University has invested a substantial sum in new laboratory construction and is similarly wisely investing in the substantial renovation of antiquated space. Chemistry has benefitted from both types of investment and has contributed by bringing external funding (both federal and alumni gifts) to some of the renovation. We will continue to look for such opportunities. In any case, given these long-term investments, we expect very little in renovation expenses for new hires.

The recent infusion of funds into acquiring state of the art instrumentation in support of the Institute for Applied Life Sciences will dramatically aid research in biomedical chemistry. It is anticipated that the recent purchase and upgrade of high resolution NMR instrumentation will help to attract top talent to one of our planned faculty hires (a hire that would otherwise command a very high startup cost). Similarly, the recent EFRC and CCI center awards allowed the purchase of state of the art equipment useful to both current and future hires. Recent faculty applicants have been impressed by our facilities.

IALS

Bioactive Delivery
Thayumanavan (steering)
Farkas
Hardy
Martin
Rotello
Vachet

Models to Medicine

Rotello (steering)
Gierasch (steering)
Chambers
Chen
Farkas
Hardy
Holden
Kaltashov
Maroney
Thompson
Vachet

Personalized Health

Monitoring
Thayumanavan
Rotello

CBI T32

Thompson (director)
Chambers
Chen
Farkas
Gierasch
Hardy
Holden
Kaltashov
Knapp
Maroney
Martin
Rotello
Thayumanavan
Vachet

Bioengineering T32

Hardy (co-leader)
Gierasch
Thayumanavan

CHM

Rotello (leadership)
Vachet (leadership)
Thayumanavan

PHaSE EFRC

Lahti (co-director)
Barnes
Venkataraman
Rotello
Thayumanavan

MRSEC

Barnes
Rotello
Thayumanavan
Venkataraman

CUMIRP - E

Thayumanavan (co-leader)
Auerbach
Barnes
Kaltashov
Kittilstved
Lahti
Maroney
Metz
Rotello
Venkataraman

Chemistry faculty: vital leaders in many centers on campus

Over the years, as computers replaced typewriters, the University dramatically scaled back staff support. In Chemistry, individual faculty now have no direct state-funded staff support, despite the large increase in compliance and accountability standards. Thus most faculty spend a large fraction of their time dealing with issues that do not require a PhD in Chemistry. The recent addition of some grant support staff in the College has helped, but is only a part of the equation. In order for faculty to be nationally competitive in the coming years, they must have additional, and targeted, staff support.

Similarly, on-line homework systems have (arguably) reduced the need for non-laboratory TAs (lecture sections were abandoned about 20 years ago). However, the management of those systems now falls directly on faculty. More importantly, as class sizes have grown and students increasingly expect more direct assistance, running a 100 student course with no TA support limits the productivity of faculty (see below) and reduces the experience of our students. Increased staff and/or TA support is essential to assure that faculty remain competitive in all that they do.

1.5 Chemistry can recruit and maintain highly successful faculty

Looking back over three decades, the Chemistry Department has an excellent track record of attracting faculty candidates who have gone on to earn tenure and continue long term, productive research careers. Indeed, of the 19 pre-tenure hires who have come up for tenure from 1990-2014, all earned tenure and all but 2 are still research active (one was active until the time of his death and another, in chemical education, left for another institution). A good number have been particularly stellar in their accomplishments, but almost all established and maintained internationally recognized, externally funded research programs. In the recent, very difficult funding climate, we have had

√ Lahti	+ Tyson
√ Jackson	√ Bianconi
√ Maroney	√ Auerbach
√ Voigtman	+ Gierasch
√ Weis	√ Thayumanavan
√ Martin	√ Barnes
√ Thompson	√ Vachet
√ Rotello	√ Kaltashov
√ Vining (<i>educ, left</i>)	√ Hardy
√ Venkataraman	√ Knapp
√ Metz	- Schnarr

Chemistry Hires 1985-2010. Check mark indicates pre-tenure hires who received tenure (+ = post-tenure hire). Those in black font have had recent federal funding

outstanding successes and some who have struggled in that climate. With the current funding climate in mind, we have established formal mentoring mechanisms, but will expand upon those in the coming year. We will continue our very successful, monthly Faculty Research Seminars, in which faculty pitch proposals to each other for constructive feedback (junior faculty always have priority in scheduling). While we have partnered junior faculty with senior faculty mentors, we will increase that effort and will establish a more formal mechanism of the pre-reviewing of draft written proposals, at multiple stages of development, to complement the Faculty Research Seminars.

1.6 The future of tenured faculty – adjustments?

As noted above, our faculty have excellent post-tenure track records in maintaining funded research programs. We have had a few longer than necessary Associate Professor residencies and will establish improved mentoring of post-tenure faculty to limit such instances in the future.

National Awards – young investigators*

Cottrell Scholar – Thompson, Rotello,
Thayumanavan, Hardy

NSF Young Investigator – Thompson

NSF CAREER – Auerbach, Metz, Venkataraman,
Thayumanavan, Kittilstved, Holden

Sloan Fellow – Auerbach

Beckman Young Investigator – Weis, Hardy

Dreyfus Teacher-Scholar – Auerbach

Dreyfus New Faculty – Venkataraman, Metz

Research Corp Innovation Award – Kaltashov

ASMS Young Investigator – Kaltashov, Vachet

Fulbright Scholar – Hardy

*pre-tenure & recently post-tenure faculty

Many of our faculty receive awards or participate in national service that provides external visibility and mentorship. Examples include the Cottrell Scholar Award, which provides not only an initial investment in a young researcher, but provides long term follow up and peer mentoring, as well as opportunities for mid-career and advanced award funding. Similarly, visiting fellowships such as the Fulbright award provide key professional development. Recent faculty have served as visiting faculty in places such as the Pasteur Institute in Paris, the Institute for Advanced Studies in Bologna, the University of Konstanz in Germany, as well institutions in Japan, the United Kingdom, the Netherlands,

China, India, Brazil, and Japan. Indeed, the University should work to encourage short term residencies or sabbaticals that involve travel, while recognizing that the modern family unit often imposes challenges that were largely non-existent 50 years ago.

Reflective of the stature that our faculty have earned, we will establish mechanisms to facilitate nomination of faculty for appropriate awards, particularly developing specific mechanisms to encourage peer support of major award nominations. We should better leverage our current successes to ensure appropriate recognition of future successes.

1.7 What would Chemistry faculty value in retirement incentives?

As outlined above, the Department of Chemistry is still suffering from the early retirement incentives of 2003. The rebuilding plan outlined in section 1.2 assumes a typical age-related estimate of retirements, with immediate replacements of anticipated retirements.

While some retirees have in the past been happy to move to non-academic initiatives in retirement, many have maintained strong and active ties to the Department. George Richason, who retired in the 1970s (and just turned 99!), continued contributing to student advising and administration for (more than *three*) decades and has served us well as an essential point of contact for very loyal undergraduate alumni. Particularly from the point of view of development, we will want to encourage similar productive visibility of key retirees. An Institute for Advanced Study (or “Academy”) would help to provide such visibility, but the regularity of faculty participation will vary with the individual. Retirees Peter Lillya and Roberta Day are examples: as key contributors to OWL development during their time at UMass, they have each continued

this development in retirement, funded by UMass' partner Cengage publishing. However, they reflect very different "desires" in retirement. Professor Day has chosen to work largely from her home in Hadley, coming to campus only when needed for consultation with collaborators. Professor Lillya very much wants to stay in touch with campus research, coming to campus daily (to work on OWL development) and requesting a (shared) office specifically near active research laboratories. While rare, the occasional retired faculty will continue with externally funded research. An example is Louis Carpino, who retired in 2004, and still maintains a small research presence funded externally (at \$200,000 in the past year) by Cem Corporation. Flexibility in space assignments will facilitate such mutually beneficial arrangements.

2. Graduate Education

2.1 Doctoral program

2.1.1 Vision for the future of the program

The Chemistry Department has been consistently innovative in education. Online web-based learning, e-exams, and iCons are just recent examples of these innovations at the undergraduate level. We similarly have a bold and comprehensive vision for our graduate education. Our innovative Core Course is one of a kind in the country for graduate students. In this course, starting immediately when new students arrive, we develop the core skills of all our graduate students, across all disciplines of chemistry, and foster collaborative mind-sets – establishing a culture early on that reflects the research in our program.

We would very much like to build on this in graduate education. Our heavy teaching needs and low tenure system faculty count have forced us to focus our recent innovations more towards the undergraduate curriculum (note that the three recent innovations from Chemistry mentioned above are all focused on undergraduate students). While e-exams are more efficient for undergraduates, OWL-type enhancements in learning (as add-ons to classroom teaching) and graduate version of iCons are critical for the graduate curriculum. We envision educating our graduate students through a curriculum that is strongly rooted in fundamentals of chemistry, as this equips them to tackle the challenges and problems that they encounter and solve in 'real life'. In addition, we also envision our students to be the next generation of leaders, who have an edge over their compatriots in other institutions. For this, in addition to the collaborative mindset, it is also critical that we cultivate a translational mindset, perhaps even an entrepreneurial mindset (at least the opportunities to do so), among our students.

The Chemistry Department graduate program attracts a diverse range of applicants, reflecting the breadth of research in Chemistry: from theoretical studies of catalysis at metal surfaces, to synthesis and preparation of inorganic coordination compounds, to single molecule spectroscopy, we attract students interested in traditional areas of chemistry. We also attract students who desire to synthesize new materials for smart drug delivery or new molecules for in vivo chemical labeling, to design proteins with novel allosteric control as potential intracellular reporters, or to study proteins embedded in natural or synthetic membranes.

The Chemistry-Biology interface: a model of modern graduate training. Chemistry faculty play leadership roles in both the well-established Chemistry Biology Interface and the new Biotechnology NIH T32 Training grants. Chemistry research laboratories frequently host students from both the Molecular & Cellular Biology and the Chemistry graduate programs, working side-by-side, and often indistinguishably. Interdisciplinarity is key to effective research and to effective preparation of students for careers in the life sciences.

Building a core materials chemistry graduate curriculum. A world-class research program requires attracting world-class research students (graduate and postdocs). Our goal is

to develop a unique materials chemistry graduate curriculum to produce next generation of materials chemists with the knowledge, skills, and attitudes needed to solve inherently multi-faceted materials chemistry problems. Our first objective will be to extend iCons Team-Based Training to graduate students in materials chemistry via 1-credit modules, plus formal research team oral and written progress and planning report evaluations. Towards this goal we will seek funding from the NSF Research Traineeship (NRT) program. Our second objective is to build partnerships with faculty from Isenberg and develop 1-credit modules that focus on incorporating economic models and design principles in materials chemistry research including concepts of materials life cycles, sustainability and scalability. Our third objective will be to revise some of the existing courses to appeal to a broad materials chemistry clientele at UMass. For example, our advanced physical chemistry courses (Advanced Quantum Mechanics, Statistical Mechanics, and Spectroscopy) are undergoing significant curriculum modifications to attract multidisciplinary students (beyond “just physical”) with an overarching emphasis on materials, nanoscience, and advanced characterization techniques. Similarly, advanced organic chemistry courses have recently focused on materials-related topics.

2.1.2 What can Chemistry do internally to improve grad student support?

A Chemistry TA is fairly demanding in its required commitments. As noted above, most students TA first and second year laboratories. Those assignments, two afternoon or two morning labs per week, plus preparation and assigned proctoring and grading, place significant time demands on a graduate student and reduce the teaching experience for themselves and for the undergraduates they teach. TA's in General Chemistry, for example, are responsible for 64 different students (undergraduates have laboratory only once every other week), limiting the personal mentoring relationships graduate TAs can have with their undergraduate students.

Despite the challenges of a significant TA load, the current teaching demands of those courses provide few, if any options to improve on the graduate student experience. Realistically, the most important thing that we can do for our graduate students is to increase the amount of external funding in support of graduate student RAs. This translates into initiatives that increase the productivity of our tenure system faculty and that increase the total number of tenure system faculty. Increasing our tenure system faculty numbers will have the benefit of both increasing the total number of external grants providing RA support and of lightening the service and (somewhat – see below) the teaching burdens on faculty, to allow them to be still more competitive in securing that funding.

When necessary, we do employ undergraduates as TAs for laboratories, however, due to their course schedules, they rarely take on two labs per week and are generally less reliable than graduate TAs (we have developed a culture within the graduate student TA ranks that they work with each other to find substitutions in the event of illness or conference travel demands – that they know each other through the first year Core Course facilitates such cooperation).

2.1.3 Preparing students for a variety of careers

Chemistry graduates find very successful careers across industry, academia and national research laboratories. Although the Department of Chemistry has a good number of graduates in academia all over the world, the majority of our graduates readily find positions in industry, in the US and world-wide. Employment of our graduate students remains very high, even at a time of economic difficulty and lack of employment opportunities for graduate students across the country. Reflecting the “interface” nature of the discipline, students are often attractive to a wide range of positions. Although we have categorized our current research in the areas of biomedical and materials research, students trained in a specific area are often attractive to careers across the board, because they are fundamentally trained as ‘problem solvers’. For

example, Dr. Rattan Gujadhur trained in DV Venkataraman's laboratory, working on copper catalysts for formation of aryl nitrogen bonds in materials research, but is now employed by Gilead Sciences, Inc, a major pharmaceutical corporation. Dr. Jason Field, also trained by DV in research on polymeric supramolecular assemblies is now President and CEO of Life Sciences Ontario, a member organization promoting Canada's life sciences companies. Eleonora Del Federico, who trained in Lynmarie Thompson's lab using solid state NMR (ssNMR) to study transmembrane sensing in bacteria, is now a professor of chemistry at the Pratt Art Institute, where she collaborates with art historians and archeologists at the New York Metropolitan Museum of Art, using ssNMR to non-destructively study pigments and materials in various media. In each of these cases, the rich interdisciplinary culture within the Department of Chemistry prepared these students well for their current positions.

Looking more to the directed placement of graduate students into careers in industry, we aim to develop more formal introductions to careers in industry. We support the Chemistry Department Student Development Committee, which organizes and sponsors the annual departmental ResearchFest each August. During this event, the Student Development Committee invites alumni for on-campus recruiting. This has been a rich means for us to place graduates in key corporate positions. In addition, we will encourage interested students to participate in the new NIH T32 training grant in Biotechnology. We will work with the leadership of this training grant (Osborn - VASCI, Roberts - ChemE and Hardy - Chem) to facilitate on-campus interviewing of chemistry graduate students by the industrial partners who will participate in the core course and other events sponsored Biotech program. We will encourage early stage graduate students to do summer internships with Massachusetts companies and will establish new graduate courses like the Applied Analytical Chemistry course that will allow graduate students to meet regularly with representatives from industry.

Finally, as noted above, Chemistry Ph.D. graduates find employment across a wide variety of sectors, from positions in industrial leadership in a wide variety of sectors, to research and/or teaching intensive positions in academia at all levels. In a Fall 2014 report in Chemical & Engineering News (volume 92, pp 12-16 - <http://bit.ly/1F9vmbp>), employment in 2012-2013 was up 3.1% for chemists overall and up 10.2% for biochemists and biophysicists (these numbers will likely be higher in subsequent years, as the economy continues to improve). The same report notes that in a March 2014 survey, "just 2.9% of ACS member chemists reported they were unemployed but looking for a job."

2.1.4 Servicing undergraduate education

The UMass Chemistry Department takes great pride in the quality of our teaching (indeed, we just added another University Distinguished Teaching awardee to our ranks), but the *quantity* of our teaching impacts both faculty, graduate students, and undergraduates, alike. Chemistry Departments nationwide typically have large service teaching demands and, reflecting the hands-on nature of chemistry, those courses require significant laboratory experience. Graduate students TAs are essential to safe and effective training in these necessarily small size laboratories (the new Integrated Sciences Building laboratories were designed around 16 student modules). As overall enrollments in these courses have nearly *doubled* in the past five years, we have met the increased need by an increase in TA resources, but have also met that need by not assigning

Fall 2014			Spring 2015		
Course	Enroll	TA	Course	Enroll	TA
Ch101	66	0	Ch101	99	0
Ch110	129	0	Ch111	290	½
Ch111	275	½	Ch111	240	½
Ch111	278	½	Ch111	283	½
Ch111	284	½	Ch112	328	½
Ch111	250	½	Ch112	306	½
Ch111	238	½	Ch112	301	½
Ch112	224	½	Ch250	89	0
Ch112	218	½	Ch261	285	½
Ch261	307	½	Ch262	300	½
Ch261	299	½	Ch262	306	½
Ch261	169	½	Ch423	62	0
Ch262	260	½	Ch476*	52	0-1
Ch341	67	0			
Ch475*	41	0-1			

TA assignment to non-lab courses.
*PChem w extensive problem sets.

TAs to even reasonably large lecture courses (see right). As a result, whereas many UMass departments assign a TA to a 50 student lecture course, our 300 student lecture courses are currently assigned a maximum of ½ TA per course and most other lecture courses currently have no TA support. Occasionally, in a course like Physical Chemistry (with enrollments of about 60-80 students and intensive quantitative and theoretical problem sets that require attentive manual grading), we are able to assign 1 TA to a course, but other courses of even 80-100 students lack any TA support at all. This lack of TA support adds to the time demands on faculty and detracts from the student experience. Thus it is essential that TA resources increase, to appropriately support our teaching mission.

A wise strategic plan logically requires a substantial investment in additional TA resources and a reduction in the typical 1:1 teaching assignment for research active faculty in Chemistry.

As appropriate to a major research University, our undergraduate majors (as well as students in service courses) benefit very directly from our top level research programs. All Chemistry majors are required to participate in laboratory research, affiliating with faculty and typically being placed under the direct mentorship of a graduate student or postdoc. Undergraduates experience a learning environment that cannot be duplicated in course-based laboratories, contribute to internationally recognized research, and are frequent co-authors on manuscripts.

Our majors course structure is being directly impacted by the evolution of research in the Department (and nationally). We are currently developing programs of “emphasis” in our major that reflect our research themes: biological chemistry and materials chemistry. The widely successful iCons program (which spans multiple departments) was inspired by our own graduate Core Course and now, the success of the iCons approach is in turn inspiring us to revisit the Core Course.

It is important to note that it is internationally recognized graduate research that distinguishes a UMass Amherst undergraduate education from the learning environment provided by many other campuses in the Massachusetts system of colleges and universities. Conversely, graduate students experience direct benefits from mentoring undergraduates, in courses or in research laboratories. The Department of Chemistry exemplifies these distinguishing features of our flagship campus.

2.2 Masters program

The Department of Chemistry does not typically offer a terminal masters degree. We have explored the idea of offering a professional masters degree, but we do not have the faculty to properly staff such an offering. Although we remain open to possibilities, this is not currently a component of our strategic plan. As our faculty numbers increase, we will revisit both this and the idea of a formal, accelerated masters degree. We would, however, want to explore the external demand for such a degree.

Appendix – Hiring vignettes in Chemistry

Structure Discovery for Functional Materials and Surfaces: We aim to hire a researcher with interests in discovering the molecular structures responsible for the functions of active materials and surfaces. The fields of materials and surface science remain very much in the dark on the complex and often disordered structures responsible for the useful properties of molecular assemblies such as drug-delivery vehicles, sensors, fuel cells, and solar cells. Developing the next generation of functional materials and surfaces requires new spectroscopic tools that can probe into the "nanoscale blindspot" – revealing chemical structures in the range of 1-50 nanometers – sizes that are too big for methods like IR and NMR spectroscopy, and too small for X-ray crystallography. Such new characterization tools offer the promise of revealing new structures of a wide array of hard and soft materials and surfaces of importance to drug discovery and delivery, chemical and biomedical sensing, catalysis, and renewable energy technologies.

Impact: Developing the fundamental expertise of structure discovery for functional materials and surface will have impacts that extend well beyond the realms of chemistry. In fact, UMass Chemistry plays a leadership role in interdisciplinary research and this hire will strengthen that position. The hire would also provide translational opportunities to industry, and provide complementary materials strengths to researchers in BMB, Microbiology, Physics, PSE, Chem Eng, and Mech Eng. The hire would also assist in re-energizing the materials science area across campus to regain our positioning in Center-based activities.

Macromolecular Dynamics by NMR or Computation: Many of the most cutting-edge questions in biological and macromolecular chemistry hinge on our understanding of the dynamics of the systems. The mechanisms of biomolecular folding, host-guest binding and responsiveness and allosteric regulation require molecular-level understanding of the dynamics of the systems. With the major upgrade of NMR facilities in progress, including two 600 MHz NMR instruments for high-level biomolecular applications to be delivered by June 2015, now is the ideal time for the Chemistry Department to make a hire that has been planned since our 2008 AQAD strategic vision: an NMR spectroscopist tackling complex, biomedically-important questions and/or a computational chemist with expertise in dynamics of macromolecules. With access to state-of-the-art NMR facilities, chemists are now uniquely placed to interrogate these systems with molecular level precision. To address such questions we seek an individual with deep NMR expertise who will develop and implement creative NMR approaches that move beyond routine structure determination of small proteins or a computational chemist focusing on molecular level understanding of macromolecular function and dynamics. This individual will complement departmental research and training in bioanalytical, biophysical, and structural biology areas and be an excellent colleague and educator in physical chemistry.

Impact: Probing dynamics by NMR or computation is an ideal complement to campus strengths in structural biology and self-assembly of nanostructures. A key feature of our campus strength in biomedical sciences is researchers with physical/chemical expertise. The desired candidate will not only understand how to use NMR to measure local dynamics, but will also have the background to interpret the data in terms of the underlying chemical interactions and mechanisms. The candidate will clearly contribute to research in the Models to Medicine and Bioactive Delivery centers of IALS (indeed, M2M has identified this as a key hire), and to training in both the CBI and Biotechnology programs. This hire would also be a resource for collaborative work with faculty across a range of life science departments, helping to bring structural biology approaches to a broader range of systems and questions, and to nucleate groups seeking funding for team projects.

Nucleic Acid Chemistry: RNA is a huge frontier research area for the 21st century. In biology, critical systems such as gene regulatory riboswitches, the CRISPR/CAS9 bacterial immunity system, and the vast cellular roles of long noncoding RNAs were completely unknown little more than a decade ago. In synthetic biology, nucleic acids are achieving the structural design goals once hoped for in protein design, including *de novo* construction of systems with tailored ligand specificity and allosteric responses.

Appropriately, we aim to hire one or more researchers in the rapidly expanding field of nucleic acid chemistry. From DNA origami in “smart” nanotechnology, to RNA therapeutics (RNAi, siRNA, et al.), to delivery of those therapeutics, a researcher developing structure-function relationships will increase the competitiveness of UMass Amherst in the biomedical sciences through his or her expertise in the creation of biomedically relevant agents and their testing using *in vitro* and *in vivo* models. With the past decade’s rapid expansion in the area of nucleic acid aptamers, which typically match antibodies in biological specificity, but are much more “designable,” the depth and breadth of potential applications is vast.

Impact: There is great strength in small noncoding RNA biology in the UMass Medical School’s RNA Institute and a growing strength in long noncoding RNA Biology at UMass Amherst. Complementing this, our Chemistry faculty are developing synthetic materials that interact with RNA, for purposes such as “smart” drug delivery. In addition to capturing the opportunities of a rapidly expanding field, this hire will have an enabling impact in all three centers of IALS (indeed, this is a targeted hire in the strategic plan of the Center for Bioactive Delivery). We anticipate that the emergent synergies would enable new research directions leading to new funding at the individual and team levels (e.g. project program grants by the NIH and the DoD medical research programs).

