Chapter 2

A Departmental Focus on High Impact Undergraduate Research Experiences

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Undergraduate research experiences have become an integral part of the Hamilton College chemistry experience. The major premise of the chemistry department's curriculum is that research is a powerful teaching tool. Curricular offerings have been developed and implemented to better prepare students for the independence required for successful undergraduate research experiences offered during the academic year and the summer. Administrative support has played a critical role in our ability to initiate and sustain scholarly research programs for all faculty members in the department. The research-rich curriculum is built directly upon or derived from the scholarly research agendas of our faculty members. The combined strengths and synergies of our curriculum and summer research program have allowed us to pursue several programmatic initiatives.

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Introduction

Undergraduate research experiences are an integral component of the Hamilton College chemistry program. We believe that the best way for students to learn science is to be engaged in well-designed, hands-on, investigative laboratory experiences that expose them to the excitement of research, ignite their interest in science and encourage them to pursue research in collaboration with faculty mentors. In the collaborative and intimate research environment, whether as part of courses or during independent research opportunities, students witness our passion for the pursuit of science and research, and mentoring relationships develop. These are the student-faculty relationships, based upon dialogue and discourse, that can powerfully influence students' decisions to pursue careers in science. Furthermore, students deemed "at-risk" of not succeeding in a science major and ultimately underrepresented in our professions — ethnic minorities, women and first generation college students — stand to benefit greatly from these close, interactive relationships (*1–4*). At Hamilton, a small residential liberal arts college with 1850 students, undergraduate research experiences exemplify the close student-faculty relationships and collaborations that we, and many small colleges, believe to be a fundamental aspect of what makes these institutions so attractive and effective.

In 1991, Hamilton College institutionalized undergraduate research by requiring an independent Senior Project of *all* its graduates. It was then, and still is, a distinctive element of the Hamilton College experience. With this campus-wide initiative came a strong commitment by the College to assist in the implementation of the Senior Project. The implementation of the program varies considerably across the disciplines and departments. For chemistry, this meant building a curriculum that prepares our majors for the independence required for a successful senior year research experience. These curricular structures have been essential to the robust undergraduate research program that now exists at all levels, not just at the senior level. Importantly, all of these structures are built directly upon or derived from the successful independent scholarly research agendas implemented by each of the members of the department.

The curriculum is the purview of the faculty and should reflect what we value most. Our department has remained committed to offering courses that provide in-depth treatment of foundational chemistry as well as explore breadth and application. The Hamilton College chemistry major is offered as an American Chemical Society accredited degree, attesting to the breadth and depth of the offerings (*5*). Within this context, we continue to experiment with ways to incorporate discovery-based learning into the curriculum, which takes shape as components of courses and laboratories, full courses and guided research experiences. In addition to the content coverage goals that we have for our various courses, we seek to address the following objectives that we believe better prepare our students for the independence required for a successful student-faculty collaborative research experience (*6*):

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- Search, read and evaluate primary scientific literature;
- Design a research project with well-articulated specific aims and a specific research plan;
- Synthesize target molecules using published protocols;
- Employ appropriate instrumentation and techniques for the characterization of compounds;
- Develop understanding of ethical, environmental, civic and safety issues associated with chemistry and laboratory experimentation;
- Communicate the nature of the chemistry and its significance.

Examples of projects that have been developed to address these objectives are included later in this chapter.

The summer research program at Hamilton has grown steadily over the past 20 years. In 1994, Hamilton College had seven undergraduates participating in summer research projects, all with faculty members exclusively from the sciences. With the support that summer of a Howard Hughes Medical Institute award, this number grew dramatically and the seeds were sown for continued growth. In the summer of 2013, over 200 students were engaged in undergraduate research experiences on our campus across many disciplines. In the Chemistry Department alone, we have had as many as 54 summer research students in a single summer and typically they number in the mid-30s. These summer research experiences are an opportunity to invite students into our research programs at a time when they are not distracted by other obligations. We currently provide students with a $400 per week stipend and offer summer housing for $28 per week. Stipends are funded from a variety of sources, including grants awarded to the institution, research grants awarded to individual faculty members, and internal institutional funds. Faculty members decide for themselves the starting dates and duration of the summer projects for their own research groups. All students participating in summer research are required to present a poster at our annual Summer Science Poster Session held during Family Weekend in the fall.

With growing student interest and active College support, a strong summer research program has become an integral part of the life of the College and the Chemistry Department. All members of the department mentor students during the summer. Significant work is accomplished during this focused period advancing the research agendas for the faculty members involved and providing significant training and experience for their student collaborators. For extended periods of time during the summer, some faculty members and their research groups travel to national laboratories where students use state-of-the-art instrumentation and interact with experts in their specific research field. In addition to the scholarly outputs that come in the form of papers published, presentations at professional meetings and research grants funded, the summer is an important time for generating momentum. One of the significant differences and inherent difficulties of doing research at an undergraduate institution is that momentum is hard to create and sustain. Attracting younger students to the summer research program provides the opportunity to build momentum and establish continuity for the laboratory, generally, and for a particular project, specifically. Many students

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choose to return in subsequent years to continue working on their projects. The summer also creates great momentum for rising seniors who will continue their projects into their senior year as the focus of their thesis research.

The summer program serves the department in other important ways. Our summer students get the opportunity to work closely with their faculty mentor and research group for an extended period of time. The formal and informal interactions that are built into the collaborative nature of the summer leads to an *esprit de corps* that develops over the course of the summer and is often carried into to the academic year. Furthermore, students are introduced to very focused research projects over the summer and often come back to the classroom with a different sense of their own role as chemists because they have had the opportunity to see the difference between studying chemistry and doing chemistry. This can have a dramatic impact on how they perform academically in subsequent chemistry courses.

Success begets further successes. The present curriculum has been established and implemented over the past two decades by the authors of this chapter and several other colleagues who have passed through our department. Support from the Hamilton administration has been essential to helping us attract and retain excellent faculty members, staff and students. The administration has also supported our program aggressively by building state-of-the-art facilities, providing support personnel for instrument methods development, maintenance and training, chemical safety and hygiene, management of our high-end computational center and a dedicated institutional grants officer. The administration has supported grant proposals with matches when needed and have responded to unusual requests that challenge standard procedures and processes. For instance, after a departmental review in the mid-90s it was clear that we needed to bolster computational activity in the department. The administration supported a senior-level hire that brought a computational chemist to our department who subsequently initiated the development of one of the best-equipped and productive computational chemistry programs at an undergraduate institution, as detailed later in this chapter. In another instance, Hamilton was awarded a $500,000 equipment grant that was spread over five years. The administration provided the required match up front so that the equipment could be purchased within the first year and a half of the grant. This enabled us to begin involving students and generating data and publications much earlier than would otherwise have been possible.

Building capacity, as happened with our computational program, is critical for a thriving department. We have continued to acquire an enviable array of state-of-the-art instrumentation through grant writing by individual members of the department. These grants have been awarded to support research and teaching objectives. Upon moving into the Taylor Science Center in 2003, the administration made the strategic decision to match any equipment request in any grant proposal at a 1:1 matching rate. This provided added incentive for faculty members to write grants and signaled to reviewers and granting agencies a significant level of institutional commitment.

The combined strengths and synergies of our curriculum and summer research program have allowed us to pursue several programmatic initiatives. The final

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section of this chapter describes some of the other programs that were initiated to attract stronger and more diverse students to Hamilton.

The Curriculum

The major premise of the department's curriculum is that research is a powerful teaching tool. This idea informs all of the courses to a greater or lesser degree, for the most part in their laboratory component. The general chemistry and organic chemistry classes still fulfill their service role, and in them attention is paid to providing the background needed to support not only the chemistry major but also needs of other science departments and of students interested in the health professions.

Originally the first two years of the Hamilton chemistry curriculum consisted of a standard one-year general chemistry course followed by two semesters of organic chemistry. However, in the late '90s, we changed the curriculum to provide a better framework for integrating research and to challenge our better students. We eliminated the laboratory components of upper level courses, except Physical Chemistry, and created a one-semester integrative, investigative advanced laboratory course. We also began awarding teaching credit for supervising senior theses. General chemistry is offered in accelerated form during the fall term, covering the principal concepts of atomic and molecular structure and bonding, thermodynamics and kinetics, general and acid-base equilibrium, and the behavior of gases and solutions. We created multiple sections of this introductory chemistry course to ensure that our students were receiving the attention they needed. The following spring and fall terms include the two semesters of organic chemistry. In the fourth semester of chemistry, students choose between introductory biochemistry and intermediate inorganic chemistry.

Introduction to Chemistry

Today beginning students have their choice of two one-semester introductory chemistry courses. The first is taught in a typical lecture format in three sections of about 35 students, with a laboratory designed with multi-week experiments that deal primarily with topics often found in General Chemistry courses — analysis of pennies, exploration of some aqueous inorganic reactions involving precipitation or not, and an introduction to chemical and acid-base equilibrium. In addition, the students work in lab groups for three weeks in the middle of the semester to design syntheses for biodiesel fuels from various sources and choose among several methods to characterize each fuel. At the end of the term, students research and carry out and present to their lab section a chemical demonstration, which allows them to begin to explore the literature and how to set up and carry out a reaction, necessary beginning tools for research.

The second introductory course is offered to students who are strongly interested in the sciences and chemistry, and is taught interactively to 25 to 30 students. We assume/expect that the students in this course have had an adequate chemistry background in high school and are ready to look at the

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broader implications of chemistry while simultaneously providing the opportunity for them to review and enhance their capabilities with the principles of general chemistry. The course now regularly includes lectures, readings and discussions on topics related to human and environmental health. The laboratory focuses on projects dealing with chemical toxicology and allows the students to hone their analytical chemistry capabilities, while assessing exposure to a variety of anthropogenic toxins. In the first half of the semester, students do directed one- to two-week projects that teach them fundamental analytical techniques. For the remainder of the semester, students work in pairs to carry out a self-designed study of contaminant levels found in some aspect of their environment. For example, students have measured levels of bisphenol A (BPA), a known hormone mimic and disruptor of endocrine function, in water bottles, cash register receipts or beer samples. They have also investigated a variety of used cooking oils or clothing for the presence of perfluorinated carboxylic acids, compounds used in the production of Teflon and likely carcinogens. In another project students examined a variety of consumer products for the presence of brominated fire retardants. One student-initiated project measured chromium and arsenic exposure from direct contact with pressure-treated lumber. The findings from this project led to the dismantling of playground structures at a local daycare facility and elementary school. The structures were subsequently replaced by units constructed of safer materials. The laboratory experience culminates with the students giving a public poster presentation on the project they have carried out during the semester. The objective of the poster session is to engage the campus community and alert them to the dangers associated with these toxic chemicals. In the course of their projects students carry out laboratory testing and do some in-depth exploration of the literature. By connecting the course material to real world chemistry students can see that the science relates to them in a significant way, which can provide strong motivation for continuing in chemistry and research. The laboratory component of this course was adopted by Science Engagement for New Civic Engagements and Responsibilities (SENCER) as one of their model courses (*7*). While this course was originally designed for well-prepared first year students, we are extremely pleased that a number of less well-prepared students are choosing this course because of the toxicology focus and are motivated to work hard to perform well in this fast-paced course.

The two-semester organic chemistry course, begun during the spring term, provides a variety of laboratory experiences that stimulate students to think about research. The sequence begins with several introductory experiments that develop students' abilities and understanding of some basic laboratory techniques. Almost all of the subsequent laboratory experiments require students to use data, obtained by hands-on use of instrumentation, to solve a problem. Students may be asked to analyze and rationalize the stereo- or regiochemical outcome of a reaction or determine the structure of an unexpected product. Students become independent in acquiring IR, NMR and GC/MS data on research grade instruments and encounter a broad range of ways in which these types of data can be used to investigate molecular structure and reactivity. For example, in almost half of the 22 labs that students do throughout the year, they will acquire NMR data on the department's 500 MHz NMR spectrometer. Although in

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many experiments, analysis of the NMR data involves standard interpretation of a proton spectrum, other experiments use integrations to determine product ratios, or analysis of coupling constant data to assign product stereochemistry or evaluation of a NOESY spectrum to define the regiochemical outcome of a reaction. Multiple exposures to instrumentation provide students with specific skills they can use in a later research experience and develop confidence in their ability to use instrumental tools to investigate scientific questions. The problem solving nature of the experiments enhances students' critical thinking skills, helps them to see science as a dynamic process and often motivates them to seek out formal research opportunities. For example, nearly 60 students, many of them sophomores, attended an evening meeting in February of 2013 in which faculty members described research opportunities for the following summer; 34 students applied.

Intermediate Level Courses

The 200-level intermediate inorganic course covers descriptive and solid-state inorganic chemistry and is often selected as students' fourth semester of the chemistry curriculum and further encourages student development in experimental design through guided independent work in the laboratory. The course enrolls a range of science majors as well as chemistry majors with an enrollment of about 30 students. Early in the lab program for the semester, students build skills in powder x-ray diffraction, as well as UV-vis, and fluorescence spectrometry through experiments in coordination chemistry, solid-state crystal analysis, and the synthesis and characterization of luminescent complexes Also included are other experiments on thermochromism, light emitting diodes, and inorganic electrochemistry. The last month of lab is turned over to the students for extended individual projects. The students each choose a project in inorganic materials whereby they are provided a basic experimental procedure that can be completed in a traditional three-hour laboratory period. Once they have performed the basic experiment, they are asked to build on the basic synthesis and characterization they carried out by proposing a series of experiments that must include the use of multiple characterization tools to explore in greater depth the synthesis or properties of the materials of their projects. Examples of the projects include the investigation of the synthesis parameters for cadmium selenide quantum dots, the effects of stoichiometry in the synthesis of rare earth iron garnets on their x-ray powder patterns, and the luminescent properties of doped zinc sulfide nanoparticles. Each project topic is chosen so that students can readily use the new methods of characterization they learned earlier in the course, specifically powder x-ray diffraction and fluorescence spectroscopy, in proposing their own experiments.

Students embrace these projects with enthusiasm and a sense of ownership that is evident when they ask for extra hours in the lab and from their presentations to the class in the final week of the semester. This makes the logistical hurdles of running 12–15 individual projects simultaneously well worth the effort. In the initial years (2006–2007), we were able to build up the basic chemicals and supplies for a wide range of projects. Each year since, we have added one or two

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new topics to the project list and we replace materials and supplies as needed. Students with more experience in the lab (for example those who had a summer research experience after their first year) need less direct guidance, but all students find that the good experimental design that must be accomplished in a few weeks is challenging. Through these projects they learn how to limit the scope of their experimental questions and design a project that provides an interesting story to present to their classmates in their 15-minute conference-style oral presentations. Some of the projects overlap in theme (e.g., properties of nanoparticles of CdS and CdSe) and so present the opportunity for students to propose parallel studies. We intentionally allow maximum flexibility in what students can propose and so often there are several new approaches to the topics every year.

The 300-level biophysical chemistry course was recently designed to be an alternative for Biochemistry and Molecular Biology (BMB) majors to the physical chemistry class required for the concentration. While BMB courses are taught by both Biology and Chemistry professors, the biophysical chemistry course is well suited for instruction by a chemist. Enrollment in this new course has ranged from six to eleven students. The course builds up three interrelated units, thermodynamics, kinetics, and quantum mechanics that lead to spectroscopy, and includes applications featuring the physical basis of biochemical properties. While the course has no laboratory component, it incorporates discovery-based learning and project design, fosters critical thinking and problem-solving skills, and teaches biophysical methods, all of which provide a strong foundation for research. Every week, students read, discuss, and present peer-reviewed research and review articles about important advanced concepts in the field.

The most research formative component of biophysical chemistry is the "mini-comprehensive" project, an in-depth study of the research publications of an important scholar in the field. Specifically, students explore physical chemistry concepts and methods in the context of the work of a distinguished professor as a common thread. During the first month, students become familiar with the professor's work and meet the professor during a video conference. Next, they work alone or in pairs to prepare a research proposal that is based on the material discussed in class as it relates to the scholar's work. They then deliver a detailed presentation of their proposed research approach and methodology to the professor who has been invited to visit Hamilton for two days. During the visit, the professor gives a seminar, meets with the students, and listens to and provides feedback on their oral presentations. This term assignment presents some challenges, including the discipline that students need to develop to work consistently on the project well in advanced of the distinguished professor's visit and the intensity of the activities during that visit. But the benefits are well worth it. The assignment requires students to digest the content of peer-reviewed articles, discuss the limitations of the methods and techniques, and understand a specific area of research in enough depth that that they can propose novel research in that area. This is learning in its highest and best form: students transfer and apply knowledge to a new area, enhancing their capacity to utilize critical thinking and analysis tools to a wide variety of situations. This helps them to acquire intellectual toughness and develop a rigorous chemistry background so they are well-positioned for advanced research.

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Superlab

The course that has been most influential on research in chemistry is "Research Methods in Chemistry" taken in the junior year and familiarly known as "Superlab." The course was originally started in the late '80s as a way of disconnecting the laboratories for the advanced courses and physical chemistry from their classroom counterparts. Because of the kinds of demands on instruction, the course was, and continues to be, taught by two instructors. In the early iteration this was a two semester course involving two labs a week plus one hour of class. In it students performed all of the physical chemistry laboratories, explored both organic and inorganic synthesis, and did a little analytical chemistry in experiments that ran for one to several lab periods. In the classroom, advanced topics, such as separation theory, ligand field chemistry, and instrumentation were touched on. In addition, attention was given to scientific writing and ethics.

In the late '90s the course was reduced to one semester, and the physical chemistry experiments were re-associated with the physical chemistry lecture courses, partly to make it easier for chemistry majors to spend a semester abroad. The course still met twice a week with one classroom period, but the laboratory experience was now built around a unifying theme with students carrying out a semester long project focused on the chemistry of metal complexes of tripodal amine ligands. Ideally, in this project students would synthesize one or two tripodal amine ligands, prepare iron and/or copper complexes of their ligands and study the properties of the complexes in the context of their ability to mimic metalloenzyme systems (*8*). Through this work, students would gain experience in the synthesis and characterization of organic and inorganic compounds, following procedures from the primary literature, and have an opportunity to explore the physical properties of the complexes. This version of Superlab, though highly successful in motivating students to carry out chemistry research, morphed into a course that placed too much emphasis on the organic synthesis of the tripodal amine ligands. Students and faculty aimed more at unknown tripodal amine ligands that promised to have different effects on the central metal ion's electronic structure and catalytic activity, and the emphasis on the complex properties and reactivity was diminished. This prompted us to find a new general research area for the course that would allow students to experience a better mix of chemical subdisciplines.

The present focus of Superlab is a semester-long exploration of the preparation, characterization and catalytic function of a group of coordination complexes using porphyrins as ligands. The course consists of three different sections. In the first, students synthesize porphyrin ligands and use these to prepare a wide variety of metal complexes. They then characterize their complexes by using different spectroscopic and physical techniques, including IR, NMR, UV-vis, Raman, magnetic susceptibility and mass spectrometry. In the middle third, working in twos or threes, the students propose and carry out a project to study an aspect of the electrochemical, ligand binding, and/or catalytic properties of the metalloporphyrin complexes. In the final phase of the semester students individually design, formally propose, and carry out an independent project.

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The course begins with all students preparing tetraphenylporphyrin. Beyond that students have control over the direction of their work with expectations of increased intellectual independence as the semester progresses. Once they have synthesized the tetraphenylporphyrin, students decide which metal ion to use to make a complex and must find a literature procedure for its preparation. For the second section of the course, students are given general guidance on what type of study to design and are provided with some seminal papers to provide background. Projects usually repeat some aspect of a published study then try to extend the study by looking at changes in solvent, substrate structure, catalyst structure, etc. Throughout these first two sections of the course, students are exploring the literature on porphyrin chemistry and begin to get a sense of the breadth of the subject. From this reading, they are expected to develop an idea for their final projects. These final projects will usually repeat and build upon some aspect of work reported in the literature but the students have the freedom to explore whatever they like. As is typical in research, some of what the students attempt works but much does not and rarely does a student accomplish all of the goals outlined for the project. One of the biggest challenges, and best opportunities for student learning, lies in the process of analyzing what is causing experiments to fail and thinking through alternative approaches, something that is difficult to teach in any way other than through a research-based experience.

The course retains a strong emphasis on working to improve student writing skills. The goal is for students to transform their writing from constructing a good lab report to producing a professional quality, journal-style manuscript. Early in the semester, the students read papers from the primary literature to see and evaluate different models of writing within the discipline. Then, on writing assignments, students get feedback through several different mechanisms including peer review, writing conferences, comments on graded first drafts and final drafts. For each section of the course, students complete a written report in journal style, the first two in the form of a note; for the last they use the style of a full paper, including an introduction with a significant literature search. They also write two proposals that describe the objectives and outlines significant background literature for their projects and present two oral reports.

In the course, scientific ethics are discussed in the context of reading Carl Djerassi's "*Cantor's Dilemma*," a novel which explores issues of scientific misconduct, politics in the academy and the difficulties women face in science, among others (*9*). Students find the novel interesting as well as a bit of a break from the intensity of some of the writing and experimentation. During the class discussion of the novel students often make trenchant and perceptive comments about both the story and the writing. These discussions often lead to extended conversations about graduate school and career options.

Superlab is challenging and sometimes discouraging for students, as they try to repeat some of the complicated syntheses and physical experiments they propose. In spite of the difficulty and attendant frustration, students find the experience stimulating and can see the progress that they make in their capabilities, often commenting on their own growth in the course evaluations. The course is also instructor intensive, which it must be, since it is like supervising eight to ten beginning research students all working on different problems. Students often

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encounter lab techniques with which they have little or no experience (working in inert atmospheres, separating compounds with column chromatography, etc.). Also, most students are unfamiliar with some of the instrumentation, like the LC/MS, and teaching them how to use the instruments properly can take a good bit of time. Working with students to troubleshoot problems and brainstorm solutions is also time consuming and can be as challenging for the faculty as it is for the students. In the end, however, the investment is well worth it. Students are enthusiastic about research and they bring to their Senior Projects and other research ventures the kind of training and background that enables their projects to move forward at a pace that can lead to publication or presentation of a poster at a national meeting.

Credit for Supervising Research

One additional recent curricular change has enabled additional research opportunities and helped to build continuity between faculty's academic year and summer research efforts. Five years ago, we instituted a new formalized course for underclass students to participate in research during the academic year. This allows them to continue research they have begun during the summer, to engage in a first research experience to see if research is something they would like to pursue further, or to get a bit of a head start on a summer project that they are planning to pursue. Students may elect to take the class for one credit, one-half credit or one-quarter credit; this is determined by agreement between the research supervisor and the student, and depends mainly upon how much time the student can afford to spend during the normal course of their semester. All faculty members in the department have worked with students through this course and an average of nine students per semester have elected to enroll.

Building Infrastructure and Capacity

Our research-focused curriculum requires two necessary and obvious components: strong research programs headed by individual faculty and high levels of student interest and participation. These programs provide upper-level students access to meaningful senior thesis projects and give underclassmen easy access to introductory projects that they can grow with. Active faculty/student research also directly adds to our curricular offerings. Keeping rigorous research programs active takes considerable effort, but an oft-repeated piece of advice is to attempt to sustain research momentum. That is, always keeping a baseline level of research productivity even at a faculty member's busiest times allows for maximal efficiency at a time when a faculty member can focus more intently on their science. By working extensively with students during the academic semesters in senior theses and independent studies, we can maintain this individual research momentum even as we have full teaching loads. In addition to this *individual* research momentum, however, our department has also recognized the usefulness of a *departmental* and even *institutional* research momentum. Individual research activity and success not only has direct benefits for the individual faculty, but

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indirect benefits throughout the department, often reaching across the campus through departmental boundaries.

A striking example of this kind of activity is the development of our college-wide, shared-use High Performance Computing (HPC) facility. To our knowledge, it is currently one of the nation's largest and most well-equipped facilities at a primarily undergraduate institution: it includes a 480-core Infiniband-connected Beowulf style computing cluster for efficient parallel processing with several large memory nodes for memory intensive calculations (e.g., *ab initio* calculations), 72 TB of redundant storage capacity, backup systems for duplication of data, and most recently, the addition of seven GPU processors to take advantage of new coding developments leveraging this powerful technology. All of these resources are available on a priority-based queuing system from student and faculty accounts mounted across a network share. This hardware and software infrastructure and the support and policies put in place to manage the resource have grown over the past decade, each advance being assisted by the previous contributions. In particular, the momentum created by past efforts has helped in securing both internal support from college administrators and external support from granting agencies.

The first contribution to the Hamilton college HPC resource was the result of a multi-investigator, intercollegiate NSF-MRI grant in 2001 that created the **M**olecular **E**ducation and **R**esearch **C**onsortium in **U**ndergraduate computational chemist**RY** (MERCURY). Significant NSF and internal funding established a shared facility made up primarily of shared memory machines useful for *ab initio* calculations. Importantly, this grant included initial funding for a full-time system administrator, a position that Hamilton agreed to continue after the NSF funding ended. This position continues to be of paramount importance as it provides the necessary linux/unix support, alleviating the technical burden on faculty since small colleges' information technology departments rarely contain this expertise. The initial success led to a second MRI grant in 2005 to expand MERCURY resources to include a Beowulf style cluster. This second MRI had a much smaller budget because the existing infrastructure enabled efficient integration of the new resources, which was probably a positive factor in reviews. An NSF-RUI grant in 2005 included an update of the shared memory computers.

Although there were personnel changes toward the end of the decade, computational chemistry remained in the department and at the College. Basic software and hardware infrastructure was in place, a dedicated HPC server room with appropriate cooling and power had been constructed, and an experienced system administrator was in place. However, perhaps even more important than these tangible advances, was the direct evidence that computational chemistry could be valuable and successful in the Hamilton College environment. This demonstration is not just important to outside grant reviewers, but to internal administrators and colleagues as well. The past success of this type of research suggests, or at least gives hope, that future successes are possible, allowing internal discussions to start at "how" to achieve certain goals, rather than "why" or even "what" those goals might be.

Successfully building computational infrastructure and integrating these techniques into the classroom and laboratories led to unforeseen institutional benefits. The analogy of all ships rise with a rising tide is applicable to this

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situation. The anthropology, biology, and physics departments each separately hired faculty with computational needs. The college recognized the broadening of this need and moved to find a viable support model. First, the HPC system administrator position, which had previously been housed within the Chemistry Department, was moved into the general information technologies structure, now serving the whole campus. Secondly, the College realized that hosting computational facilities in each lab needing such resources would result in redundant duplication of services and be an inefficient use of space, time, and money. Therefore the College committed to a shared-use, College-wide computational facility to combine services general to all groups, e.g., data storage and backup, queuing and authentication, etc. To organize these various computational groups, the administration created an *ad hoc* committee, called the "HPC Governance Group," to manage the resources and set policies concerning their use. At first, the Chemistry Department was hesitant to agree to these changes. The system administrator position and the facilities themselves, previously under the department's direct control, would now be managed at the College level. However, the positive effects soon became obvious. The research momentum created by the success of computational chemistry had helped the administration recognize the value of the activity, and more importantly, the need to support it. The system administrator had the scope of his activities increased to support faculty outside of the sciences, most notably a burgeoning Digital Humanities Initiative (DHI), but his main focus still lies with HPC. And now that HPC is viewed as a campus-wide activity, rather than the focus of a single investigator, the administration has been more willing to commit significant resources to it. The Information Technology department committed two computational nodes to a new computational chemist's startup in addition to the normal Dean of Faculty support, it added 96 (20% of our current total) modern computational cores in exchange for shutting off older machines that operated with much higher power consumption, and, when our data storage reached its capacity, it added 20TB of additional disk space for the HPC users.

While the legacy of Hamilton College computational chemistry certainly helped our administration understand the possible payoffs of investment in this type of activity, current active and productive research programs are critical to ongoing support. The new chemistry faculty hire primarily utilizes classical molecular simulations that require efficient parallel computation but requires very little memory, different from the demand on the original cluster. To add the type of hardware necessary, faculty from chemistry, anthropology, biology, and physics applied for and were awarded an NSF-MRI with the title: "Acquisition of a High Performance Computing cluster with a fast interconnect to enable shared-use, college-wide computational investigations at Hamilton College." The title makes clear the evolution in support models at Hamilton. One of the proposal's main arguments was the efficiency with which it could utilize NSF's investment given the expertise and infrastructure already existing on campus. This grant funded 288 of our 480 total cores. An additional individual Research Corporation Cottrell College Scholar Award funded an additional 96 cores.

The College's commitment to a shared-use model has continued throughout each of these contributions. Although a principal investigator has priority access

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to the equipment, any Hamilton College faculty member or student can gain access to use the HPC facility. This is important to continuing the momentum that computational research activities have enjoyed at Hamilton College. Because of the open access to our HPC facility, faculty from Africana studies (through the DHI), anthropology, biology, chemistry, economics, geosciences, mathematics, psychology, and physics have used the HPC facility or its expertise. While only a few of the investigators have directly contributed resources to the facility, the larger and more diverse number of users strengthens the argument both internally and externally for supporting HPC activities. Much as efforts at the beginning of the millennium helped enable our successes at the end of its first decade, we hope our efforts will sustain the institutional momentum for computational research at Hamilton College for the foreseeable future.

Building on Success

There is significant collateral good that can come from a robust undergraduate research program. Three programs in particular are described in this section that benefited directly from the research environment that exists in our department during the summer include: 1) Pre-matriculant Research Experiences, 2) Hamilton College-Paris VI Exchange Program, and 3) Hamilton College - Oneida Nation Summer Research Program. Each of these is built on the premise that once our individual research programs are up and running in the summer, we can bring others into the program for shorter research experiences. The students benefited directly from the research momentum and camaraderie within the department.

Pre-Matriculant Research Experiences (*10*)

This program was originally designed to attract students to Hamilton and the sciences by inviting all students accepted for admission to Hamilton to apply for the program that would allow them to spend five weeks during the summer prior to matriculation working on a research project with a faculty member. Selected students joined research groups in mid-summer following their graduation from high school. Evidence suggests that some students not selected to participate in the program ultimately chose Hamilton because they knew they would have other opportunities to do this sort of research. The program was funded with grants from the NSF-Science Talent Expansion Program (NSF-STEP) and the Camille and Henry Dreyfus Foundation's Special Grant Program in the Chemical Sciences with the explicit goals of attracting more majors to the sciences and improving retention. Funds were used to pay students a $350 per week stipend (equivalent, at that time, to the stipends paid to other summer research students) and students were housed together on campus using a learning community model. In addition to their pre-matriculation summer experience, the College funded a 10-week summer research stipend for all students who participated in the program to return to campus during a subsequent summer. By all measures, this program was an overwhelming success. During the four year grant period, 75% of the

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participants majored in a science discipline with greater retention and graduation rates than the non-participants.

Hamilton College – Paris VI Exchange Program (*11*)

Hamilton has had a very successful study abroad program in Paris for many years. Mostly for logistical reasons, the program had trouble attracting science students. Students participating in the program could ostensibly take science courses at University Pierre et Marie Curie (University Paris VI), but there was no formal mechanism for the program to compensate Paris VI for the spot these students would be taking away from French students. An exchange program was created in which Hamilton College would accept Paris VI students for a summer research experience and students in the Hamilton Paris Program would be able to take courses at Paris VI.

The program is an excellent cultural exchange experience for the French visitors to our labs and for our students and faculty members. The Paris VI students are academically very well prepared, having completed coursework comparable to Masters level work, so they possess a rich understanding of the background science underlying the projects they work on in collaboration with Hamilton faculty members. However, many have never had research experience nor been exposed to open-ended, inquiry-based pedagogy and so have much to learn in the laboratory. By contrast, the Hamilton students are very comfortable navigating within the research laboratory with a mature sense of experimental design. They can design and execute the experiments but, with less formal training and the language barrier, the breadth and depth of their understanding is not as advanced. It has been truly a rich collaborative effort in which all participants bring different strengths to the experience.

Hamilton College – Oneida Nation Summer Research Program

Hamilton College has had a long relationship with its neighboring Oneida Indian Nation. In fact, the College was originally founded to serve the children of Oneida Nation families and white settlers and was named the Hamilton-Oneida Academy. This relationship lay fallow for many years. With a small grant, we began to provide two-week summer research opportunities to Oneida Nation high school students. The program was coordinated with the Oneida Nation Education Department who helped to select participants. The goals for the program were modest. We simply sought to provide an opportunity for these students to spend time on a college campus. Native Americans remain the most underrepresented of all ethnicities in higher education. With little community tradition and few role models, these high school graduates approach college with great trepidation. Our goal was to show them that there is a place for them on a college campus.

We designed the program such that Oneida students would work on projects as teams with a faculty mentor. Following the research experience, Hamilton hosted the students and their families for a tour of the science building to see and hear about their students' research projects. The students also presented their projects to the Nation Council, where they were enthusiastically received.

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We were thrilled when two of the program participants matriculated at Hamilton. One graduated as a neuroscience major and was awarded a Fulbright Teaching Assistantship upon graduation from Hamilton.

Concluding Remarks

Undergraduate research has blossomed at Hamilton College in the past 25 years. The model now includes disciplines in the social sciences, the humanities and the arts, as well as the sciences. The broad success of the model confirms the assertion that research is a powerful teaching tool. But as this chapter implies, the development of the focus on research through the departmental curriculum and the dedication to having students in our labs year-round have far-reaching implications. By having a common purpose, the department can work more effectively together. As a consequence, the administration is more willing to provide support and outside granting agencies take note. Other departments see the appeal of the program and find ways of incorporating ideas from it into their own departments in a manner that suits their philosophy. The department itself garners increased respect both from within and without the college. Ultimately, however, it is the students who gain the most. The skills that they develop through a challenging curriculum and through collaborative research experiences make them highly sought after by graduate and professional schools and more competitive for national awards. Providing an effective education and helping to open up opportunities for our students is, after all, our primary goal.

Acknowledgments

Developing and maintaining an effective department requires time, effort and a willingness to work collaboratively among the core faculty and the authors of this chapter are grateful to one another for their commitment to excellence. The success of the department depends on so much more than the work of the core faculty, however. We would like to acknowledge the work that many colleagues do to enhance our work. These include Steve Young, the system administrator for the computational center, Shawna O'Neil and Anne Delia, our current and previous Director of Laboratories, and Mary Collis who is the Building Coordinator for the Taylor Science Center. We have also benefitted from working with many other faculty colleagues through the years, both tenure-track and visiting, who are no longer with us, including Tim Chapp, Camille Jones, Josh Ruppel, Nicole Snyder, Ram Subramaniam, Jack Waas, and Brad Wile. Our students also play a critical role in making their own educations successful and we are fortunate to get to work, year in and year out, with a wonderful group of intelligent and motivated students.

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