

Report of the Ad Hoc Faculty Committee on Molecular Engineering

February 14, 2007

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Executive Summary

The environment for research at the molecular level is undergoing a paradigmatic shift that involves the blurring of traditional boundaries between the basic and applied sciences and engineering. This shift will have profound consequences for the nature and practice of molecular-level science in the coming century. Molecular engineering concerns the incorporation of synthetic molecular building blocks including electronic, optical, mechanical, chemical and biological components into functional systems that will impact technologies from advanced medical therapies to quantum computing. We have examined the question of whether the University should explore and, if the resources can be raised, create a new research component in Molecular Engineering. We find, after extensive consultation with the faculty, that there are compelling reasons for the University to move in this direction. Moreover, we have considered the consequences of not taking this action. The University's research enterprise and education mission will undoubtedly continue to flourish at the highest international level, but the consequence of inaction in this area of endeavor may well abdicate activity in some of the most promising new directions of physical, biological, and medical research. We acknowledge that the establishment of a Molecular Engineering unit represents a large undertaking for Chicago, but one with tremendous possibilities to position the University as an intellectual leader in this emerging engineering discipline. Moreover, such action will undoubtedly provide new partnerships and routes to discovery for our faculty in the basic molecular sciences, enabling them to continue to define the horizon in their respective fields of research.

Overview

The ad hoc faculty committee on molecular engineering was constituted to assess whether the University should create a new unit in Molecular Engineering that would complement our already vital and internationally distinguished activities in the basic physical, biological, and medical sciences. The motivation for undertaking this assessment at this time is that a paradigm shift is underway presently, where the boundary that once separated the basic sciences (the study of natural phenomena) and engineering (as the development and study of man-made artifacts) is blurring, especially for research involving systems at the molecular level. This changing research landscape challenges the traditional models for Engineering departments and raises profound questions for the optimal organization of the research enterprise at institutions that aspire for world-leadership in this area of endeavor for the next century. Chicago must carefully consider the consequences of remaining different from virtually all of its peer institutions in this regard as the decision whether to establish, or not to establish, such an entity in the applied sciences and engineering will have tangible consequences for the scope and direction of research at the University in the coming century.

The committee has consulted broadly with the faculty and has hosted widely-publicized town hall meetings with the faculties of the Biological and Physical Sciences Divisions. We have also considered the relevant strengths that follow from our evolving research relationship with Argonne National Laboratory.

We find that there exist compelling intellectual arguments for the creation of a new element in the University's research portfolio, Molecular Engineering. Moreover, it can be argued that not taking this step at this time will place the position of world-leadership we presently hold in the basic physical and biological molecular sciences at risk due to the rapid evolution that is occurring in these forefront areas of research. Systems engineering at the molecular level is in its infancy. The creation, control, and hoped for societal impact of such systems will require a strong and synergistic partnership between the basic and applied sciences with related engineering disciplines.

Our enthusiasm for this action is tempered by an important caveat: in order for this initiative to succeed it will require a significant and long-term institutional commitment of human and financial resources - with success being clearly defined as the creation of a new group of engineers and applied scientists on campus who will rise to a position of elite intellectual leadership in partnership with the University's extant excellence in the basic and medical sciences. We believe the goal to be attainable with commensurate and enduring commitment from the University.

The Need for Engineering

Research and teaching in the natural sciences and engineering disciplines have historically shared little overlap. The natural sciences have excelled in revealing the principles by which physical and biological systems operate and the engineering disciplines have brought this knowledge to the realization of methods and devices that solve real-world problems. This clean separation between basic principles and applications has blurred, and in many areas, an integration of basic science and engineering approaches is now common. Indeed, studies in the sciences routinely require sophisticated apparatus that are designed and built by engineers - for

example, multielectrode arrays that are used to study neural tissues and electronic device technology to package displays and electrical circuits prepared from organic polymers. Moreover, advances in engineering often lead to observations that motivate studies in the sciences: examples include studies of surface forces in MEMS devices (the Casimir Effect), modulation doping and the quantum Hall effect in semiconductor devices which garnered two Nobel Prizes in physics, formation of ultra-cold matter on microchips with applications in quantum computing, and massively parallel approaches to drug discovery and probing cellular function, and myriad applications of molecular level imaging and manipulation derived from engineering advances in electron, confocal, and specialized scanning probe microscopes (the direct observation of molecular conformational changes and the forces associated with such transformations). This increased collaboration between the sciences and engineering disciplines is correlated to a shift in project funding from the traditional single investigator model to co-investigator efforts. A significant and still growing fraction of the research portfolio at the NSF, NIH and other agencies is targeted towards multi-investigator efforts that emphasize both problem-solving and basic science. We believe that this trend will continue and will make it increasingly difficult for universities with outstanding science departments, but an absence of engineering, to remain leaders in the traditional sciences.

Why Chicago/Why Now?

We find that the field of molecular engineering, at this early stage of inception, is well matched to the culture and strengths of the University of Chicago. The last two decades have undergone an explosion in the knowledge of molecular systems – the routine and mundane collection of that information was largely not a focus of our institution, but was rather left to service-oriented facilities. Meanwhile, institutions that invested in large-scale engineering efforts have focused on moving ever closer to the molecular scale. Today many cutting-edge achievements in engineering no longer require capital investments in large-scale prototypes for industrial processes. Consequently, there is ample opportunity for an innovative organization such as the University of Chicago to tap accumulated molecular knowledge and, in a cost-effective manner, design small-scale solutions that will be at the forefront of engineering advances. Doing so requires a nimble institution that can draw on the expertise of the physical and biological sciences and merge that talent toward practical solutions.

There is a critical time when key, empowering discoveries and technical developments lead to revolutionary rather than evolutionary advances. The high-tech world of electronics made such a leap when vacuum tubes were globally replaced by their solid-state counterparts, driven by the advent of the transistor, integrated circuit, and solid-state memory. One theme common to this and arguably many branches of engineering has been miniaturization: electrical engineers seek to reduce the size of the transistor; mechanical engineers build mechanical devices at smaller scales; and aeronautical engineers are building micro aircraft and studying fluid flow in nanochannels. As each of these disciplines approaches the molecular length scale, the top-down approaches used to fabricate devices and the continuum models used to understand the devices break down, with a clear understanding that new strategies in fabrication (bottom-up strategies that employ synthesis and self-assembly) and in molecular modeling are needed. It is significant that these approaches have been developed and are widely practiced in the sciences (chemistry, physics, and biology). Indeed, today's engineering departments increasingly seek junior faculty with backgrounds in the sciences.

Realizing this vision is going to require the kind of innovation that is central to the culture of the University of Chicago. Faculty members of the University are problem solvers – they recognize deficiencies and think “out of the box”, often combining solutions from different disciplines. It has been said that most innovation arises from the application of the principles of one discipline to the problems of another. The close-knit nature of the campus and faculty at the University of Chicago catalyzes these kinds of breakthroughs – compared to many other institutions, where a long commute is required from biology to chemistry to physics to medicine – the University of Chicago’s compact campus facilitates serendipitous collisions of ideas. There are numerous examples of cross-disciplinary collaboration as a result. Consequently, our campus is often the birthplace of ideas that change entire fields.

Rapid cycling from the laboratory to the real world and back to the laboratory is tremendously beneficial, and often the key to developing technology to a point of practical utility. While many campuses have invested in this activity, they have traditionally separated innovation and execution into basic sciences and schools of engineering – these separate efforts evolved their own traditions and distinct cultures such that they find communication challenging. At the University of Chicago, we have an opportunity for a better approach by harnessing the inspiration of our innovative faculty, and by adding a group of individuals who are willing to engage those innovators, we can blend culture, disciplines and approaches toward the innovations that will reshape our future.

Stated clearly, Chicago has a clean slate with respect to the traditional engineering disciplines and the infrastructure of the last century. We do not need to participate in the ongoing refinement of fifty meter tall catalytic crackers in the chemical industry or follow the Edisonian paradigm of materials discovery. We can forego these efforts, and leapfrog into the 21st century by focussing on the creation of new knowledge and move rapidly into the next forefront area of molecular systems based upon expertise in complex systems, bottom-up methods, self-organization, biomimetics, along with their natural complements in theory and numerical simulation. We have the proper intellectual foundation in the physical and biological sciences to partner with a new engineering element in molecular engineering to bring Chicago into a position of intellectual leadership in this still-being-forged engineering paradigm of the coming century.

Intellectual Opportunities

Molecular engineering represents a tremendous opportunity for the University’s entrée into engineering. Molecular engineering concerns the incorporation of synthetic molecular building blocks such as electronic, optical, mechanical, chemical and biological components into mesoscopic and/or macroscopic functional systems. Intellectual opportunities are abundant and diverse. Moreover, traditional categories of field compartmentalization readily breakdown when considering molecular-level systems. Profound lessons from the working of biological systems will undoubtedly inform advances in the physical sciences, with the converse being equivalently true. Many scientific and technological advances will in fact involve hybrid systems involving organic, inorganic, and biological components. With this in mind, we herein suggest a few broadly-conceived themes that are ripe for exploration and development, and that can be used as illustrative examples of where a molecular engineering effort may focus its efforts. These topics

have been chosen as worthy challenges in the Chicago tradition as they offer the promise of intellectual importance, broad and lasting impact, and, with lots of hard work and some good fortune, broad-ranging opportunities for societal impact in the physical, biological, and medical sciences.

Suggested initial themes include:

- Systems engineering at the molecular level
- Energy conversion, transport, and storage at the molecular level
- Understanding and controlling complexity and self-organization at the molecular level
- Imaging, sensors, and transponders for probing and controlling molecular level systems
- Molecular-level electronics and device fabrication
- Advanced polymeric and hybrid materials
- Assembly of nanoscale systems for physical, biological, and medical applications
- Information storage, persistence, and retrieval in physical and biological molecular systems
- Biomimetic Systems and Materials

We of course acknowledge that this is only one (but very well-conceived!) list of the coming high-ground in the area of molecular engineering – the lead hires in this engineering initiative will, in addition to exploring some of these themes, undoubtedly move into unanticipated and worthy new directions, precisely the intent of bringing to the University a new cohort of investigators with fresh ideas, new tools, and a complementary perspective to our already world-class efforts in the basic sciences. If done properly, this will undoubtedly bring immense benefit to our efforts in the basic physical, biological, and medical sciences.

Synergies with the Basic Sciences at Chicago

Assisting this launch will be natural and very powerful research elements that are already in the University's research portfolio. Our strengths in physical, materials and synthetic chemistry; biochemistry; condensed matter physics; neurobiology; molecular genetics and cell biology; large-scale computation; and medicine are a subset of the disciplines that provide the enabling environment for nucleating a new engineering effort, and, in turn, stand to directly benefit from the establishment of a research arm in molecular engineering. We find pronounced synergies with many of our traditional departments in the Physical Sciences and Biological Sciences Divisions, especially those that have as their foundation the molecular sciences. Moreover, we also have a powerful cohort of interdisciplinary Research Institutes, Committees, and innovative multi-investigator federal grants that will play a key role in welcoming Molecular Engineering to campus and in helping to weave it into our highly-interactive and cross-disciplinary research milieu.

Illustrative scientific themes (not an exhaustive list!) that are already part of our research portfolio and that have obvious synergies with molecular engineering include:

- Assembly of molecular and hybrid organic-inorganic functional materials
- Biomimetic design of functional materials
- Molecular electronics
- Polymer synthesis, design, and device engineering
- Nanostructures and self-organization

- Protein engineering
- Complex, integrative systems of cell signaling
- Synthetic chaperones
- Nanomedicine
- Molecular imaging and sensors
- Synthetic biology

Clearly, investigators in each of these areas would benefit from the presence of experts in engineering at the molecular scale. But more importantly, having such experts on campus would likely prompt the blossoming of interests among BSD and PSD investigators whose current work would benefit from extension toward molecular engineering but who have not attempted such forays previously because of insufficient opportunity.

Consequences of Inaction for the Basic Sciences

Given the strong and growing interconnections between the basic and applied sciences and engineering at the molecular level there is also a strategically important downside that must be acknowledged should the University choose not to establish the proposed unit in molecular engineering. In the near future, the University may lose access to some of the most innovative young scholars in the basic and applied molecular sciences. This matter of faculty recruitment and retention can be summarized into four categories: (i) currently, we miss opportunities to hire excellent researchers whom we do interview because their research programs look too different from the core missions of extant departments, (ii) we do not interview those with a clear engineering vision who would empower our basic sciences with needed technology and further enrich the milieu for discovery at Chicago, (iii) some recruits with programs in the molecular sciences whom we do want accept positions at peer institutions with engineering elements as we do not have the right environment to grow their programs, and (iv) science is changing – Chicago faculty who work at the boundaries of the basic molecular sciences may depart to peer institutions that do offer the engineering elements necessary to take their already successful programs to the next level.

With respect to medical research it seems clear that Chicago could fall behind its peers were it not to develop novel engineering science. For the most part, medical disease happens at the molecular level, and our interventions to reverse it (treatments) are aimed at the molecular level (e.g., small molecule drugs target protein domains, etc.). To fail to adopt or perform research to advance new technologies toward these goals is certain to disadvantage the BSD.

Synergies with Argonne National Laboratory (ANL)

The recently enhanced relationship between the University and Argonne National Laboratory will provide several key benefits to Molecular Engineering. Solving the big problems in molecular engineering will inevitably require the formation of diverse teams and access to unique large-scale capabilities available at Argonne such as the molecular-scale imaging capabilities at the Center for Nanoscale Materials (CNM), the Consortium for Nanoscience Research (CNR) – a joint UC-ANL initiative in nanoscience, the Advanced Photon Source and the Electron Microscopy Center, the synthesis and nanofabrication capabilities at the CNM, and the computing resources that are poised to exceed 100 Teraflops. Relevant programs in the Material Sciences, Chemistry, and Biological Sciences Divisions at ANL will offer other routes

to productive research. Mutually advantageous (and occasional) joint appointments with Argonne may also arise with this new initiative, further augmenting its engineering impact and scope. However, the desire for such joint appointments should not be allowed to mitigate the advantages we perceive that come with the University's "clean slate" in engineering, i.e., Molecular Engineering must be allowed to launch and evolve its program in optimal fashion, forming alliances with Argonne when warranted by its own programmatic needs.

Molecular Engineering Education

Engineering Education: Establishing degree granting programs in Molecular Engineering is important for the University's growth. Engineering is the science of solving complex problems. The tools of engineering are important in translating basic discoveries in other fields into useful technologies. Therefore, strengthening engineering research and establishing engineering education would strengthen the University's ability to serve society.

Because of the breadth and strength of existing research in molecular engineering, the graduate educational programs leading to MS and PhD degrees would be developed first. The didactic curriculum could be organized within one year. Students entering this graduate program would need a quantitative science background. This background would be augmented by graduate courses in applied math and physics, synthetic and physical chemistry, materials science, imaging, computational methods, statistics, among other topics to be planned and tailored to individual needs. The opportunities in molecular engineering that exist on campus and at Argonne National Laboratories are robust and would readily support excellent opportunities for doctor thesis research. Within three years an undergraduate program could be developed that would draw from existing courses and require newly developed courses. Models for this curriculum exist at several other prominent universities that have established applied science and engineering schools.

With a focus on molecular engineering, baccalaureate and masters degrees in Engineering Science or Applied Physics would not fall under the auspices of ABET (Accreditation Board in Engineering and Technology) certification because it is unlikely that many students entering these programs would pursue careers in traditional engineering disciplines such as civil, electrical, mechanical or other traditional engineering fields that often require state board certification for independent engineering contractors and consultants. Rather, matriculates will become research scientists, business leaders, patent attorneys, etc.

Impact on other Programs: The introduction of engineering education at Chicago would have broad impact on the University's programs across all divisions. As repeatedly stressed in this report, forefront research in the basic physical, biological, and medical sciences is presently undergoing revolutionary change with respect to critical linkages to the applied sciences and engineering. We must strive to educate our students with the critical skills they will need to become tomorrow's leaders. To do this, they must be exposed to an appropriate and broad palette of basic science *and* technical engineering skills, especially for research at the molecular, nanoscale, and cellular levels. If done properly, we can be assured that future breakthroughs in the basic biological sciences and medicine in critical fields such as drug discovery, genomics, proteomics, and cellular dynamics will continue to flow from our researchers. Similar impact in

the physical sciences will also occur, with training in molecular engineering enabling our studies on such diverse topics as nanomaterials, molecular electronics, complex systems, and energy.

Examples of Successful Initiatives Elsewhere

One question that can be asked is whether, in today's hyper-competitive environment for physical, biological and engineering research, institutions can successfully grow new broad-reaching programs that achieve positions of leadership on the national and world stage. Examples do exist. These recently created entities share common characteristics: a clear and absolute commitment of the institution, a visionary leader who executes the institutions' aspirations for excellence in the chosen area of endeavor; a lead scientist of elite international reputation from inside or from elsewhere who may or may not have been the visionary cited previously; the financial resources to execute the programmatic launch; and in many instances lead senior hires, as individuals or groups of researchers, from other institutions around whom other recruits would nucleate as they decided to join the building effort. Examples come from many directions.

The recent explosion of activity in Nanoscience gives three powerful creations: the *Smalley Institute for Nanoscale Science and Technology* at Rice University, the California NanoSystems Institute, and the London Centre for Nanotechnology (a joint venture between University College London and Imperial College London). JILA (formerly known as the Joint Institute for Laboratory Astrophysics) is another unquestioned example of such a success. It is arguably the lead research institute in the world in the area of atomic, molecular and optical (AMO) physics. The success of these institutes can be clearly linked to two key ingredients: a visionary, world-renowned leader and substantial institutional investment. Other successful launches can be cited from the biological sciences. Two excellent ones are The Scripps Research Institute in La Jolla and the new Janelia Farm campus for the Howard Hughes Medical Institute. Finally, we note the Max Planck Society runs an extensive network of research institutes which are created around forefront issues in science and technology. The two brief case studies given below, one each chosen from the physical and biological sciences, illustrate the preeminence that can be achieved in a generation with a well-conceived vision of excellence and direction.

JILA was launched some time ago (1962), and has become one of the world's elite centers for research. In partnership with NIST, and with a faculty of 33, it is home to three Nobel Laureates and two MacArthur Fellows. Its launch also had its visionary, Lewis M. Branscomb, who steadily accumulated a remarkable ensemble of researchers with complementary interests in the chemistry, physics, and astrophysics. Recent achievements include breakthrough discoveries in ultra-cold matter (Bose-Einstein and Fermi condensates) and precision laser spectroscopy. The Scripps Research Institute focusses on basic biomedical science, and has grown to become one of the country's largest, private, non-profit research organizations. In just three decades it has established a lengthy track record of major contributions to the betterment of health and the human condition. Particularly significant is the Institute's study of the basic structure and design of biological molecules; in this arena TSRI is among a handful of the world's leading centers.

Organization and Scale

The committee has given considerable thought to the organization and scale of proposed activities in molecular engineering. For Chicago's new effort to have significant impact we

believe that a target faculty size of 24 is an appropriate goal. This size would be sufficient to host a broad range of activities in the physical and biological aspects of molecular engineering (and certainly many of these activities will by their very nature bridge interdisciplinary boundaries). These researchers could, in our considered opinion, be initially organized into four to six theme areas, with the lead senior hires, perhaps two per theme, helping to identify those who would follow. This would be the scenario for the launch. If we hire the right people, they will take the enterprise into the most promising new areas, many likely unanticipated at this time by this committee.

A crucial aspect will be autonomy for Molecular Engineering. It will need to set, after partnering with extant faculty for the initial launch, its own engineering research agenda. This will ensure that it can develop properly, and not be subject to hiring constraints imposed by the traditional basic science disciplines. For this purpose, we envision a department-sized effort, perhaps being administered as a School. A School has the advantages of independence of budget, hiring, and space with respect to extant elements of the University.

What factors help to set the scale of such an endeavor beyond its programmatic themes? Realism dictates that the proper financial foundation must be in place for this to succeed. This will be discussed in the following section on resources and infrastructure. Another consideration is the time the University will allow for the launch. The goal of making the necessary hires to properly launch four or six theme areas could be realistically achieved in a decade or less including the construction of key infrastructure. If successful, further growth could then be added on in fractions or multiples of the initial ensemble.

We note that many world-leading research entities are of the proposed scale. As example we cite the activities in atomic physics at JILA (on the campus of the University of Colorado at Boulder and joint with NIST). Its faculty currently numbers 33. We also note that the University of Chicago Law School, arguably one of the most distinguished elements in the University's research portfolio, has 26 full-time faculty members.

Resources and Infrastructure

Molecular Engineering will require substantial resources if it is to be properly launched and achieve success. Our *conservative* estimate is that a minimum of \$250M will be required for its launch and growth. This figure obviously depends on the initial scale. This figure includes endowment to support faculty and staff (\$100M), a new building to hold research labs and common facilities (\$75M), common facilities for biological and physical research (\$25M for clean rooms, microscopes, lithography, tissue and cell culture, computational resources, etc.) and \$50M for faculty recruitment. Space allocations may average 2,500 sq ft per investigator, with lead faculty requiring substantially more than the average allocation. Depending on focus and ambition, the size of the building may need to be expanded beyond the present estimate. Leveraging of assets already present on campus and at Argonne National Laboratory should help moderate costs, a factor already taken into account in our guideline. Proximal access to unique instruments such as the Advanced Photon Source may also be expected to play a role in faculty recruitment for researchers who value and need its specialized capabilities.

Our committee wishes to add an important caveat to this section of the report: This initiative, regardless of its final scale, will be expensive. It should not be launched without the proper financial foundation and enduring University commitment that will be needed to make it internationally competitive at the highest level of aspiration. To do so will risk failure. Moreover, given the importance this initiative will potentially have on the intellectual evolution of extant Departments, a poorly executed launch would likely lead to commensurate problems in presently world-class Departments and Institutes. On the other hand, proper execution of this initiative has a tremendous upside for the University, including the creation of an engineering component that independently, and in concert with traditional efforts in the basic sciences, will reshape Chicago's research landscape for the coming century. It may well ensure that Chicago has the complement of intellectual resources that will be needed to continue to hold its position of leadership in many fields that depend on excellence in the basic molecular and biological sciences.

Respectfully submitted for the Ad Hoc Faculty Committee on Molecular Engineering,

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