DEPARTMENT OF CHEMISTRY STRATEGIC PLAN

Chemistry is ubiquitous. Chemistry is reality. If we are to ultimately understand everything around us - air and water and earth and buildings and cars and desks and paper and ink and trees – that understanding will derive from chemistry. Sight and taste and smell and touch, themselves, are chemistry, as is the motion in a muscle and the emotion in a mind. Life is chemistry. But chemistry does not merely seek to uncover nature's secrets. Whether it is generating new materials and pharmaceuticals, or inventing new reactions, or simply synthesizing molecules that test scientific ideas, chemistry builds things. It is a science of both understanding and invention.

Nanoscale materials, smart polymers, molecular diagnostics, gene sequencing, lamellar waste filters, medicinal natural products, sensor arrays, biocatalysis, molecular machines, atmospheric photoreactions, nerve agent detoxification, archaeological analysis, biosynthetic engineering, spintronics, drug delivery – the forefronts of each of these areas and many more are under study in the Department of Chemistry at Texas A&M University. As the central science, chemistry is both an outlet for advances in mathematics and physics and the foundation for biology and medicine and engineering. The opportunities in chemistry are endless, as are its frontiers of fundamental knowledge. A hundred years from now, chemistry will be new, chemistry will be thriving, chemistry will be important to its sister sciences.

Texas A&M University epitomizes the promise of land-grant institutions to serve as ladders of social mobility, engines of the state economy, and the very stalwart institution that our communities rely on to meet their needs for the ever-advancing front of human knowledge. Since its inception, the Department of Chemistry has remained true to the land-grant mission of Texas A&M University. The Department has played a central role in advancing foundational science in the service of humankind and in underpinning the emergence of the State of Texas as an energy powerhouse. In these unprecedented times, buffeted by crosswinds of a global pandemic, a rapidly evolving landscape of economic opportunities, depleting natural resources, and generational challenges at the food—water—energy nexus, the Department of Chemistry at Texas A&M University aspires to emerge as a global leader in the Chemical Sciences. The Department of Chemistry has a long-standing history of excellence in research and teaching, consistently ranked within the top 10 among public institutions in the US. Our faculty boasts 11 Distinguished professors (including members of the American Academy of Arts and Sciences and the National Academy of Sciences) and is recognized for a strong commitment to education, highlighted by two Presidential Professors of Teaching Excellence, and a commitment to outreach as evidenced by our long running Chemistry Open House and the Chemistry Road Show, which enhances STEM education across the State.

Building on its past, and inspired by its future, the Department of Chemistry used the SOAR (Strengths, Opportunities, Aspirations, and Results) framework to formulate a strategic plan that both fuels and defines its research trajectory over the next decade. In addition to fulfilling its scientific ambitions, this strategic plan will also guide future investments, including those defined during the 2020 Academic Program Review (APR). The most urgent recommendation emanating from this APR included the hire of 25 faculty over the next 10 years, not just to buffer anticipated retirements and university growth, but to match our aspirations for leadership in the global scientific community. Another important conclusion of this APR was the creation of state-of-the-art space to realize these ambitious goals. Against this backdrop, the Department of Chemistry at Texas A&M University has identified **four research thrusts** that have foundations in current strengths but also are designed to expand its research profile to address future global challenges and opportunities, while enhancing its educational mission and paving the way for new synergies within TAMU and with core external partners invested in our success: **Chemistry for the Expansion of the Human Frontier, Chemistry of Life, Chemistry for Sustainability, and New Lenses on the Chemical World**.

CHEMISTRY FOR EXPANSION OF THE HUMAN FRONTIER

Vision and Goals

TAMU Chemistry seeks to develop a fundamental science playbook that will support the resilience of communities and infrastructure in the face of natural disasters and anthropogenic extreme environments, while enabling an unparalleled exploration of economic opportunities on this planet and others. As such, our vision is to develop strengths that bring us into a perfect alignment with the space and sea grant missions of Texas A&M and to be pioneers in the fundamental science of human exploration and habitation in extreme environments.

Turning the adverse changes affecting our world into opportunities, the Department of Chemistry at Texas A&M University aspires to emerge as the global leader in the *Chemistry for the Expansion of Human Frontiers to Extreme Environments*. By exploring chemistry away (including far away) from equilibrium and from ambient conditions, we seek to develop a new atlas for chemistry in extreme environments ranging from the deepest ocean floors to farthest reaches of space. We seek to develop a fundamental science playbook that will support the resilience of communities and infrastructure in the face of natural disasters and anthropogenic extreme environments, while enabling an unparalleled exploration of economic opportunities on this planet and others. As such, our vision is to develop strengths in Chemistry for the Expansion of Human Frontiers that bring us into a more synergistic alignment with the space and sea grant missions of Texas A&M and to be pioneers in the fundamental science of human exploration and habitation in extreme environments.

Several factors make this a particularly opportune time for a significant effort dedicated to developing a transformative fundamental science toolkit for addressing extreme environments. The tantalizing possibilities afforded by these factors inspire our priority areas: (***a***) the cislunar economy and chemistry in deep space; (***b***) the need to encode resilience as a fundamental design principle in coastal and low-lying communities in the face of natural and anthropogenic disasters such as Hurricane Harvey and the Deepwater Horizon spill; (***c***) the evolving nature of combat across air, land, and sea; and (***d***) an unprecedented race for scarce critical resources. Addressing these challenges will require in depth research expertise spanning traditional and emerging areas of chemistry, inculcating into our research enterprise an unprecedented agility, and the ability to rapidly scale discoveries along the technology development continuum in tandem with strategic partners. The proposed area builds on core departmental strengths in understanding chemical design principles and chemical transformations at extremes of temperature, salinity, pH, redox potential, concentration gradient, pressure, acceleration, and exposure to intense bursts of energy; nationally leading prowess in radiation testing and radiation-hard materials; extensive capabilities in decoding metabolic processes and the rules of life under extreme conditions; and deep expertise in the design of metastable soft and hard materials. On a 5—10 year horizon, through faculty expertise, staff, and distinctive infrastructure, the Department of Chemistry will establish global leadership in (i) in developing design rules for predicting chemistry far away from equilibrium, transcending longstanding bottlenecks in the prediction, rationalization, and realization of chemistry outside of thermodynamic minima; (ii) designing and manipulating molecules, materials, and cellular processes to enable exploration and habitation of extreme environments; and (iii) reimagining the fundamental building blocks of infrastructure to build resilient communities protected from the effects of natural disasters and climate change. The department will have in place institutionalized mechanisms of nimbleness, scale, and partnerships that will serve as a national model for chemistry performed at breakneck speeds in response to evolving needs and crises.

Potential for Transformative Impact

The department will build global leadership in deciphering design rules away from equilibrium. This will be accomplished by collating faculty expertise that brings together distinctive experimental methods and simulation approaches and combining it with distinctive infrastructure—a fully equipped modular chemistry maker space—that can be operated at full capacity in times of turmoil and crises. Through the development of unprecedented models for academia—state—federal collaborations, we will be the fundamental science powerhouse that drives the aspirations of the Great State of Texas for energy independence, novel economic opportunities, sourcing of critical materials, and exploration of human frontiers deep below the surface, at geographic extremes, and in deep space. We seek to launch a new paradigm that embraces the opportunities provided by extreme environments and situations and to harness their potential instead of simply seeking to mitigate their impact. In addition to expansion of human knowledge, the societal impacts of this enterprise will include access to critical resources needed to sustain and grow our quality of life and the economic benefits inherent to such exploration, resilience of populations and infrastructure in the face of natural and anthropogenic extreme events, and understanding of the fundamental origins of life.

Potential for Synergy (at TAMU and with External Partners)

At TAMU, the cyclotron has nationally leading capabilities that will play a pivotal role in radiation testing and space readiness. The Army Futures Command being established at the RELLIS campus further affords unprecedented opportunities for fundamental and translational research related to hypersonics. The Center for Infrastructure Renewal at RELLIS is furthermore rapidly emerging as a nationally leading center for evaluation of soft and hard materials under extreme conditions. San Antonio military labs ((Army Institute of Surgical Research, AF 59th Medical Wing, NAMRU-SA) provide opportunities for biomedically aligned research of relevance to combat readiness. The recent partnership with Los Alamos holds promise for exploration of opportunities in all of these areas and allied fields.

Primary synergies include the NASA Johnson Space Center and JPL (building on some initial conversations), private space entrepreneurs, defense contractors such as Lockheed Martin and Northrop Grumman, the many large Houston-area energy companies, and industries directly affected by materials criticality such as the electric vehicle (e.g., Tesla's recently announced manufacturing initiative in Texas) and wind power supply chains. The Texas State Chemist's office could further be a medium for facilitating a much larger role in reflecting the aspirations of the state for economic growth and job creation through addressing the challenges outlined in the preceding sections. A major need in the area is to establish an infrastructure that allows TAMU faculty to be plugged into emerging opportunities and to respond rapidly to evolving needs. There is an urgent imperative for seamless TAMU/TEES collaboration across the entire spectrum of activities outlined above.

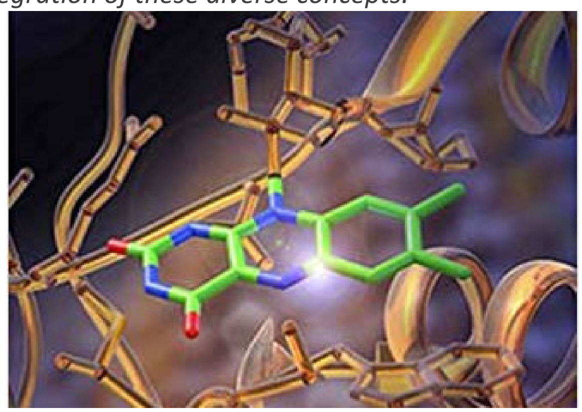
Impact on the Educational Mission

Given the overarching themes of resilience, space exploration, and combat preparedness that underpin this thrust, distinctive opportunities exist for engaging student veterans, including under the auspices of the Hazelwood program, Corps of Cadets, and students interested in careers in the armed forces. The research themes further hold opportunities for interdisciplinary workforce development in emerging areas such as coastal resilience, cislunar economy, space health, and deepwater resource extraction.

CHEMISTRY OF LIFE

Vision and Goals

TAMU Chemistry embraces the Chemistry for Life as a concept that encompasses all elements, whether essential for life or used to understand and improve life. In doing so, and building on the solid and far reaching tradition that we have established in the multifaceted field of biological chemistry, our department will assume a global leadership founded on the holistic integration of these diverse concepts.



The application of chemical methods to the solution of biological problems is now a highly sophisticated branch of chemistry that has a broad impact on the life sciences. The chemical understanding of living systems impacts every area of modern life. It includes the design of useful new compounds as drugs, imaging agents, and biomaterials to combat disease; the development of synthetic and enzymatic chemistry to maintain a healthy living environment; and molecular probes to enhance our understanding of the chemical basis and evolution of life. Building on our wide-ranging strengths in the chemistry of biological processes, we map out our research trajectory for the next 5-10 years, focusing on four areas at the frontiers of "The Chemistry of Life".

With global warming and population growth increasingly displacing animals from their native habitats, zoonoses are likely to become even more threatening and frequent. At the same time, increasing pollution levels, industrialized food, and the unthinking application of synthetic materials is making our world more toxic, leading to a host of diseases. Capitalizing on our existing strengths in the chemical biology of diseases, we will position ourselves to address the adverse consequences of these macroscopic changes. Combining approaches from synthetic organic chemistry and chemical biology, Texas A&M Chemistry will become a powerhouse for the design, screening, and testing of lead compounds as antibiotics, antiviral, and anticancer agents. Our efforts will lay the foundation of therapeutic strategies that can be rapidly deployed to tackle the ever-growing list of diseases that affects humanity. The agility of our response to these challenges will hinge on our continued dedication to the creation and advancement of fundamental knowledge in the broad area of the “Chemistry of Life”. As such Texas A&M Chemistry will foster a an all-inclusive and, at-time, out-of-the-box approach to the topic while at the same time assembling a large cohort of the finest minds in the discipline who will discover new molecules and explore fundamental processes in cell biology using imaging agents, molecular sensors, and omics probes. These efforts will be leveraged by advances in the development of new drug delivery strategies using porous solids, polymeric nanomaterials, and cell-specific/penetrating peptides. In keeping with our fundamental research mandate, we will seek to understand the modes of action of all newly discovered antibiotics, antiviral, and anticancer agents at the cellular level. In turn, we will continue to expand our understanding of cellular chemistry through mechanistic studies that will characterize the biological pathways, including enzymatic ones that are essential to maintaining health. Over the next decade, we intend to continue these successful research efforts and acquire new strengths in four research areas: a) developing diagnostic tools for disease biomarker detection; b) developing new strategies for imaging in disease diagnosis; c) synthesis of physiologically active complex natural products for biological target identification; and d) developing innovative chemical techniques for basic and translational research in the life sciences.

Given the solution to pollution is chemistry, we, as members of the global chemistry community, view it as our primary responsibility to invent and deploy strategies than mitigate the consequences of human activity. Our vision for the future includes a thrust by which we will unleash the power of the “Chemistry of Life” against the accidental release of fracking fluids, oil spills, and greenhouse gases using bacteria that will catabolize these organic pollutants both in the soil as well as in our water resources. Advances in bioanalytical strategies will serve to assess the effectiveness of our mitigation strategies. At the same time, the isolation of the bacteria that degrade organic pollutants/microplastics and the characterization of their enzymatic machinery will provide a molecular-level understanding of their catabolic properties, ultimately allowing for their optimization. Advances in the field of bacterial metabolism will cross-fertilize with our desire to harness the human microbiome for the production of metabolites that enhance human health and prevent/cure diseases. Our strengths in natural products, biosynthesis, and enzymology are an ideal stage to launch a major thrust in this new research area of direct relevance to human health. Transporting our knowledge from the human gut to the Petri dish, will help us define new chemical biology strategies for production, by fermentation, of drugs, vitamins, and other useful metabolites.

Potential for Transformative Impact

Over the next 5-10 years, our goals are to continue to make significant contributions to our understanding of "The Chemistry of Life" and, in so doing, increase our research productivity, funding levels, and our national ranking. Coordinating "The Chemistry of Life" research across traditional areas of chemistry will give us unique strengths and synergy as a chemistry department, enhance the recruitment of top-tier faculty and graduate students and stimulate stronger interactions with the other life science departments. Our active engagement with state health and environmental problems will strengthen our relationships with the Texas biotechnology and chemical industries.

Potential for Synergy (at TAMU and with External Partners)

The chemistry of life is developing from a molecule making discipline to a molecule design-synthesis-testing discipline. As we continue to embrace this evolution, it will be essential for chemistry of life researchers to form increasingly close relations with the Departments of Biochemistry and Biophysics, Biology, Molecular & Cellular Medicine, Veterinary Medicine, and programs such as the Synthetic and Systems Biology Innovation Hub and the Toxicology program. We are making good progress in building these important relationships, and a number of our faculty have joint appointments that have fostered strong research collaborations.

Biotechnology is a robust commercial enterprise in Texas and offers an abundance of collaborative research opportunities over a wide range of life chemistry problems (Texas Biotechnology Company directory, https://businessintexas.com/wp-content/uploads/2020/ 06/biotechdirectory.pdf). We will put a greater effort into exploring these opportunities, including the possibilities for short-term internships for our students. We will reach out to industrial partners for the commercialization of our research on enzyme functional assignment, enzyme engineering, and biosynthetic pathway characterization.

Texas also has several premier biomedical research institutions (UT Southwestern, MD Anderson, Texas Medical Center). We will leverage our proximity to these institutions and to the Texas A&M’s Health Science Center for the translation of physiologically relevant research to the clinic. Recently our faculty have initiated discussions on collaborative projects with the Texas Medical Center. Such projects have the potential to transform research at TMC which lacks the strong chemistry infrastructure required for promoting translational development of diagnostics and therapeutics.

We will explore the possibility of collaborative projects on the biodegradation of microplastics, fracking chemicals, and petroleum with Haliburton. We will also seek advice on Texas's most pressing environmental problems from the Texas Commission on Environmental Quality.

Impact on the Educational Mission

The chemistry faculty play a central role in the education of life science students. While our traditional chemistry teaching has provided these students with a solid foundation for understanding the chemistry of biological systems, the continuous rapid evolution of the life sciences now requires major changes in the traditional teaching mechanisms and course content to incorporate the chemical basis of new concepts and techniques. Vibrant junior faculty recruits will play a key role in curricular development by integrating new research concepts into their teaching.

We will expand opportunities for cutting-edge education in the chemistry of life with new hires and continue developing new courses to foster the molecular understanding and analysis of biological systems. Computational chemistry and machine learning methods will provide a key interface for a new generation of omics that seamlessly blends *in vitro*, *in vivo*, and *in silico* experiments. The broadening of our research activities will also require that our students increasingly take relevant courses in biochemistry, biology, environmental science, and engineering.

We anticipate developing stronger collaborative relationships with chemical and biotechnology companies in Texas by having students in "The Chemistry of Life" program participate in complementary internships with these companies. We are confident that an interdisciplinary approach to graduate student training in "The Chemistry of Life" will result in the recruitment and training of outstanding young scientists. We view this research focus as a suitable area by a NIH training program.

The centrality of chemistry to the design of materials impacts virtually all economic sectors, from advanced computing, to energy storage and production, to personalized medicine. By developing predictive, robust approaches for chemical synthesis, that are greener, more energy efficient, and that truly take advantage of the ability of chemistry to reform materials atom-by-atom, we seek to democratize the landscape of chemical synthesis, by enabling chemistry by design, on demand, opening the door to unprecedented new technologies and advances that restore the planet.

CHEMISTRY FOR SUSTAINABILITY

Vision and Goals

The judicious use of resources is central to the sustainability of our society. Whether it be the development of processes that use less energy (e.g., catalysis); the ability to reclaim and recycle or upcycle materials; creating materials that can capture and/or store energy; developing approaches for removing environmental waste (e.g., water purification/storage); or the design of synthetic processes that produce less waste, while providing more economically feasible pathways for making materials, sustainability is a core principle of chemistry, now and for the future. Within our department we have significant strength in each of these areas that we can also build on, with the vision of Chemistry at Texas A&M University, leading Texas, and the nation, in research and education in sustainability within the next decade.

Potential for Transformative Impact

Sustainable Polymer Chemistry. Our faculty have significant breadth and strengths in the application of theoretical, computational and experimental techniques for the development of biological and chemical approaches to contribute to two primary initiatives toward sustainable plastics – dealing with existing petrochemically-derived micro- and macroplastics that persist in the environment and designing new sustainably-sourced degradable polymer materials. In one direction, we seek to advance the fundamental understanding of chemical principles and processes that lead to the transformative outcome of developing strategies for recycling mixed plastic waste and economically transforming such waste into original feedstocks for value-added products. In another direction, enzymatic and chemical catalysis is being studied to transform biomass into building blocks, which paired with the development of synthetic methodologies for their transformation into sustainable polymers, enable their breakdown into regeneratable natural products. Our efforts are defining chemical parameters and associated transport phenomena that involve single and multiple substrates to understand and master polymer deconstruction/reconstruction, with the goals of minimizing energy and economic costs, while maximizing yield, and ease of integration into the sociopolitical landscape. Exploring multifunctional materials that take advantage of natural polymers, and clays, and other biorenewable resources, as well as approaches for leveraging methane, CO and CO_2 as synthetic feed-stocks brings our efforts full circle to establish our department as a leader in sustainable soft matter. Moreover, moving forward, teams involving chemists and engineers have been assembled to study polymer materials that are designed to address flooding, drought, and other effects of climate change.

Catalysis. Our department's core strength in inorganic chemistry, and the ability to tailor new catalysts through ligand design, remains of paramount importance. This work translates to the design of biologically-inspired enzymatic catalysis, as well as the use of benign environmentally friendly oxidants. Recently, TAMU Chemistry has been awarded an NSF Centers for Chemical Innovation grant, to launch the *NSF Center for the Mechanical Control of Chemistry* (CMCC). The CMCC will serve as a world-wide locus for a unique set of nano- macro-scale metrologies and models that will enable researchers to directly probe and understand the effects of mechanical force on diverse chemical reactions. CMCC's understanding of mechanochemical reactions will inform the evolving sustainable chemistry community, where mechanochemistry affords greatly reduced solvent use/waste, safer and more energy-efficient synthetic methods with lower processing temperatures, faster processing times, and completely new synthetic routes for materials including pharmaceuticals. Across each of these catalytic systems, translating the atomic-scale view to the macroscale has the potential for substantial technological and economic benefits globally.

Materials for Energy Capture and Storage. There are growing efforts directed toward energy generation, conversion and storage, which are of critical importance to fuel the future of society with protection of the resources of our planet. Here, TAMU Chemistry has been focused on the pursuit of materials for hydrogen and methane storage, taking advantage of the rich chemistry of cutting-edge materials with ultrahigh porosity which continue to develop not only for the energy landscape, but also for environmental remediation through methane and CO_2 capture, with possibilities for sequestration of chemical waste materials. Along with these areas, a building effort on the design of materials for energy conversion has emerged centered around the unique properties of nanostructured materials, including oxides for more efficient batteries, hierarchical organic molecules, perovskites and quantum dots, for light harvesting, and plasmonic materials for enhanced light-matter interactions.

Advanced Materials for Sustainable Computing. Transmitting, storing and processing data already accounts for ~10% of global energy use; extrapolations indicate that by 2040, demand for computation will be 10× higher than the projected global energy supply. Here, chemistry will seek to have a transformative impact by developing materials for brain-inspired computing, to identify, understand and leverage unexploited physical phenomena giving rise to strongly nonlinear dynamical changes of electrical conductance, realizing functionality of neurons (thresholding, integration and action potentials) through materials science and enabling a million-fold improvement in efficiency and speed of computation over current technology.

Potential for Synergy (at TAMU and with External Partners)

Our transformative innovations in sustainability will continue to be fostered by strong industrial collaborations (e.g. Dow Chemical and Eastman Chemical Company) to translate our fundamental work into practice. Here the formation of strong industrial consortia would aid in support this endeavor and we will seek to emerge as the key solution provider for the chemical and petrochemical industry in the State of Texas and beyond. In TAMU, key partnerships with the departments of Materials Science and Engineering, Statistics, Electrical Engineering, Biomedical Engineering, Biochemistry and Biophysics, and Geoscience, as well as the Energy Institute and the Data Science Institute, will allow us to launch forward into translating the fundamental understanding of materials and chemical synthetic mechanisms that underpin sustainability into key applications that impact society. This effort will be further supported as we engage more and more computational efforts and machine learning to guide materials synthesis and design.

Central to our success are also essential partnerships with national labs. Many faculty already work with Lawrence Berkeley, Sandia, and Los Alamos and growing partnerships with Pacific Northwest, Argonne, and the National Renewable Energy Laboratory are on the horizon. Formation of a more coordinated national labs partnership network (in conduction with the TAMU system National Labs Office) will be enabling for our research activities.

Impact on the Educational Mission

What is clear from the research directions denoted above is that the growing importance of convergent research also requires correspondingly dynamic and responsive educational plans that can not only provide the cross-cutting backgrounded needed for our students to push these areas of research forward, but also as a means to best prepare them for their future careers. In the area of sustainability, this entails the development of a robust internship program with industry and national lab partners, which many undergraduate and graduate students are looking for. The additional interactions with industry should also be supported by robust integrative courses in entrepreneurship and innovation in partnership with the College of Business, McFerrin Center for Entrepreneurship and School of Innovation. Enhanced interactions and curriculum development with the Bush School of Government and Public Service will also be pursued to educate our Chemistry students in public policy, of importance to the chemistry of sustainability for our planet. Modular coursework that involves innovative online and peer instruction mechanisms will also foster a stronger educational community that many students crave. Tied in with our already strong undergraduate research experience programs, senior design and team projects will aid in developing the work ethos sought by employers and would increase our competitiveness for recruiting the best students from across the State of Texas and across the nation at all levels, in alignment with the land-grant mission of Texas A&M.

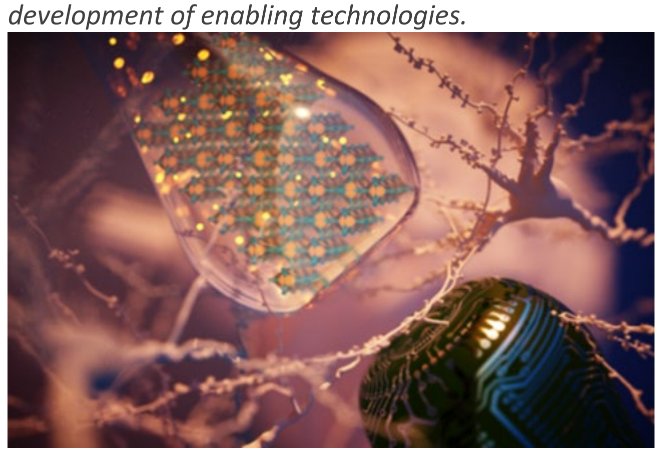
NEW LENSES ON THE CHEMICAL WORLD

Vision and Goals

What can be more central to the pursuit of scientific knowledge than understanding the fundamental building blocks of matter, atoms and molecules, and finding ways of manipulating them to the benefit of Earth and its inhabitants? Our abilities to observe atoms and molecules as they make and break chemical bonds, assemble to form molecular machines that initiate or inhibit disease, and the myriad of processes that define environmental conditions related to climate change are the ultimate objectives of chemistry. Enabling technologies capable of expanding our atomic/molecular vision of chemical processes occurring on ultrafast time scales, in non-equilibrium systems, in living biological systems, and interstellar space play a central role in our ability to understand our place in the universe, decipher the origins of life, decode the complexities of the living world, and intervene as needed to combat disease, improve our quality of life, and mitigate the catastrophic effects of climate change.

Disruptive progress in understanding molecular assemblies in different environments requires breakthroughs in analytical instrumentation and methodologies, which will unite and span across the "*Chemistry for Expansion of Human Frontiers to Extreme Environments*", "*Chemistry of Life*", and "*Chemistry for Sustainability*". Our goals are to build upon the rich history of analytical/physical chemistry at TAMU in discovery and development of enabling technologies.

Enabling technologies capable of expanding our atomic/molecular vision of chemical processes occurring on ultrafast time scales, in non- equilibrium systems, in living biological systems, and interstellar space play a central role in our ability to understand our place in the universe, decipher the origins of life, decode the complexities of the living world, and intervene as needed to combat disease, improve our quality of life, and mitigate the catastrophic effects of climate change. Progress requires breakthroughs in analytical instrumentation and methodologies, building upon the rich history of at Texas A&M in the discovery and development of enabling technologies.



As an exemplar of our past and present, we foresee an accelerating momentum in the area of native-mass spectrometry and its application to structural biology. Through these efforts, we will gain unprecedented insights into the structure and assembly of protein complexes and even viruses. The unparalleled cutting-edge capabilities already present at TAMU will serve to investigate challenging and dynamical protein systems, such as those embedded in lipid bilayers. These capabilities will be complemented by advanced imaging mass spectrometry capabilities adding to other structural biology resources such as in high magnetic field NMR, cryo-electron microscopy and molecular dynamics simulations. Collectively, these capabilities are poised to elucidate mechanistic insight for molecular-level understanding of proteins function, including how other molecules regulate their function.

Another important aspect of our vision will bring to bear cutting-edge surface science and super resolution ultrafast visible and IR microscopy as integrated tools to interrogate a host of materials systems ranging from 2D materials catalysts to individual proteins. Further advances in surface analytical toolsets will be deployed to mechanically control chemistry in a range of projects that integrates high spatial resolution microcopies with *in situ* Raman and IR spectroscopy. Photoelectron spectroscopies will serve to monitor the progression of surface chemical reactions as they proceed. These toolsets will be paired with high-end computational efforts to match experiment, with a key direction of implementing machine learning to advance our understanding of surface chemistry. Advances in these future capabilities *in situ* electron microscopy capabilities to explore chemical reactions for the synthesis of nanomaterials.

Investments in theory and computation will be pivotal to harnessing the power of simulations to accelerate discovery, augment chemical intuition, and develop closed loop cycles of molecular and materials innovation. Building upon a long tradition and extensive infrastructure of high-performance computing, we will ensure that modeling and simulations are integrated with every aspect of the chemical sciences spanning the range from the development of new theoretical methods to quantum chemical descriptions of fundamental chemical processes, largescale simulations of the dynamics of charge, energy, and mass transport in biological and materials systems, and the use of machine learning and deep learning to uncover hidden correlations and develop intuitive chemical understanding.

Potential for Transformative Impact

Future needs in areas of enabling technologies and methodologies are amply documented by granting agencies, National Academy of Science reports, mission statements of national laboratories and documentation from high-tech companies. A number of Nobel prizes and other prestigious awards have recognized transformational advances in measurement sciences. Advanced technologies have contributed greatly to solutions of longstanding chemistry questions, discovery of new chemical processes, Advanced technologies have contributed greatly to solutions of longstanding chemistry questions, discovery of new chemical processes, identification and development of new drugs and vaccines and even in vitro/in vivo diagnostics. Research in cancer and solutions to our current pandemic and numerous other human health conditions lie in the development of therapeutics and vaccines, a chemistry problem that hinges on key technologies used for testing and development of new drugs/vaccines.

While TAMU is heavily invested in analytical chemistry, chemical instrumentation and related enabling chemical measurement technologies, the challenge is to create tomorrow's measurement infrastructure. Currently missing is a competence in instrument design to develop technologies that are the game changers and critical differentiators. They will provide a competitive edge across the chemical enterprise at Texas A&M. Being able to "see" processes occur in their natural environments and to be able to articulate design rules will provide an unmatched advantage to synthetic chemists and chemical biologists and will allow their imagination to be channeled into purposeful discovery and innovation.

Potential for Synergy (at TAMU and with External Partners)

Building world-leading analytical and computational capabilities at Texas A&M University will not just provide our entire chemical enterprise with a competitive advantage but will have widespread resonance across the entire university and the research ecosystem of the State of Texas with compounding effects that will uplift the regional economy. Chemistry can play a central role in university-wide initiatives in data sciences. Key synergies include deep knowledge of the foundations of artificial intelligence in Statistics and Math within the College of Science as well as Texas A&M's Institute of Data Science. Establishing leadership of the analytical "omics" revolution will be key to alignment with the statewide mission of the Cancer Prevention and Research Institute of Texas and the Texas Medical Center—the largest medical enterprise in the world. The development of cutting-edge spectroscopy tools will enable leadership of hypersonics research, a key thrust of the Army Futures Command initiative on the RELLIS campus. The challenges of developing advanced enabling technologies are coupled with scientific curriculum initiatives at RELLIS.

Impact on the Educational Mission

Analytical and physical chemistry play central roles in education and maturation of students independent of their primary area(s) of interest(s). Synthesis, characterization and identification of new materials all require advanced knowledge of the basic tools of qualitative and quantitative analytical techniques, and the concepts and principles of physical chemistry serve as the underpinnings of modern chemistry. Nowhere is this more apparent than in biological, materials and nanochemistry where samples are obtained in extremely small quantities from complex matrices and oftentimes comprising a subunit of a molecular complex. The challenges of modern chemical research also extend beyond isolation and/or synthesis of molecules—solutions to the problem(s) require highly interdisciplinary approaches, both in terms of the chemistry and the tools used to decipher the molecular-level information. While the above amply describe the challenges our students experience in their research, it is unfortunate that our teaching program remains “old school” and dissects the materials into the single domain. The transition to a problem-solving and interdisciplinary teaching structure will be challenging, but it is essential that we do so. We will reimagine our undergraduate laboratory curriculum to tear down silos and to place inquiry-based learning, authentic research practice, and discovery at the heart of the Aggie undergraduate experience.