SCIENCE ALLIANCE

2019/20 Annual Report

THEC State Appropriations Request 2020-2021

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EXECUTIVE SUMMARY

The Science Alliance remains a foundational partner in fostering relationships between the University of Tennessee, Knoxville, and Oak Ridge National Laboratory (ORNL). Our researchers have consistently engaged in meaningful collaborations with ORNL researchers for more than 35 years, and recent partnerships in the areas of advanced manufacturing, exascale computing, and neutron science highlight some of the unique capabilities afforded by the scientific climate in East Tennessee.

In FY20 the Science Alliance launched several new programs in keeping with its recently developed strategic plan. The Support for Affiliated Research Teams (StART) program supported innovation within the greater research enterprise by prioritizing projects with first-time collaborations between UT and ORNL scientists or new applications of established expertise. Additionally, the unification of the University of Tennessee, Knoxville, and the University of Tennessee Institute of Agriculture (UTIA) allowed the Science Alliance to extend these opportunities to previously ineligible faculty members.

The Science Alliance has a proven history of supporting graduate students at the university. The Student Mentoring and Research Training (SMaRT) program began its first full cycle of joining UT undergraduate students with graduate student mentors in preparation for a summer research work experience. Despite the challenges associated with COVID-19, the campus community came together to find new and creative ways to engage with students and continue their research.

In June 2020 the Graduate Advancement, Training, and Education (GATE) program released its first call for applications. The program will provide 12-month graduate research assistant opportunities for high-achieving graduate students to further develop their research beginning in August of this year.

In addition to the flexibility and determination exhibited by Science Alliance–funded researchers, the Science Alliance deployed a rapid response funding opportunity through the Joint Directed Research Development (JDRD) initiative to boost research on campus with potential applications to address the COVID-19 pandemic. Funded projects began in August 2020.

In keeping with its historical spirit of collaboration, the Science Alliance enacted an advisory board in 2020. The board is composed of UT and ORNL scientists and administrators, with the purpose of ensuring open lines of communication between the Science Alliance and the local research community and further promoting transparency between the unit and its stakeholders.

Impacts of the COVID-19 pandemic have been felt in academic institutions across the nation, including the University of Tennessee. The Science Alliance worked hard during this time to maintain programmatic and research capabilities at UT, despite the necessary closing of ORNL to guests. We are now poised to complete the launch of our strategic plan, including a number of programs that will enrich faculty and student opportunities across campus and at ORNL.

This report is more than a summary of the research activities of our Distinguished Scientists, StART Fellows, project leaders, and students. In these pages you will find stories of resiliency and innovation, the development of new collaborations, and the bolstering of academic achievement across a variety of disciplines. Science Alliance awards are an investment in the university, its faculty and students, and the competitive future of the state of Tennessee.

Shawn Campagna
Faculty Fellow for Research Development
Interim Director of Strategic Programs for ORI@UT

SCIENCE ALLIANCE OVERVIEW

The Science Alliance is a Tennessee Center of Excellence, established in 1984, and supported annually by the Tennessee General Assembly.

The mission of the Science Alliance is to:

- Hire and support joint distinguished scientists of national note
- Create and support joint institutes
- Share resources
- Bring the University of Tennessee and Oak Ridge National Laboratory together to support technology transfer
- Build areas of common strength
- Provide incentives to attract and retain the highest quality faculty and students
- Strengthen educational opportunities
- Grow government and industrial support of the shared research enterprise.

Science Alliance funding is one critical way that the partnership between UT and ORNL is further advanced. Funds support a variety of significant investments in people and collaborations.

Much of our current collaborative research emphasizes strategic areas of importance to both organizations. Advanced manufacturing, advanced materials and materials science, neutron science, computational science, big data and data science, and bioinformatics are currently among the most prominent UT-ORNL collaborative areas receiving support.

The investment made by the state each year in this important collaboration is greatly appreciated and is instrumental in allowing the Science Alliance to provide a variety of opportunities for innovative and groundbreaking collaborations between people. Great science and discovery come when people-to-people interactions are optimized, not unlike a chemical reaction. A reaction progresses because of interactions, and these funds support those interactions. They hold a decisive role in leveraging the federal investments made at ORNL and UT in our areas of collaborative research and development.

MISSION STATEMENT

The Science Alliance

was established in 1984 to improve selected science programs at the University of Tennessee, Knoxville, and to increase collaboration between the university and Oak Ridge National Laboratory (ORNL).

The Science Alliance is composed of four divisions, the original three being **Biological Sciences, Chemical Sciences,** and **Physical Sciences**. A fourth division, **Mathematics and Computer Science**, was added in 1986.

Science Alliance objectives:

- Create a strong formal bond between UT and ORNL
- Hire joint UT-ORNL distinguished scientists
- Create joint UT-ORNL institutions
- Share resources and build areas of common strength at UT and ORNL as well as with industry and other institutions
- Contribute to technology transfer
- Provide incentives to attract and retain high-quality faculty
- Strengthen graduate and undergraduate opportunities
- Increase public and professional awareness of UT-ORNL partnerships

GOALS AND FUTURE PLANS

Since its inception, the Science Alliance has been tasked with creating opportunities for meaningful collaboration between the University of Tennessee, Knoxville, and Oak Ridge National Laboratory (ORNL).

The Science Alliance has worked to achieve this goal through the creation of programmatic opportunities for faculty, students, and research scientists for over three decades. In the past year, a new strategic plan was implemented to continue and expand upon these efforts. In addition to the existing Joint Directed Research Development (JDRD) program, a number of new programs were implemented to further enhance the relationship between the university and ORNL.

The Support for Affiliated Research Teams (StART) program, launched in November 2019 FY20, provided faculty members with up to two years to explore first and new collaborations with ORNL researchers. Projects that receive awards are required to produce an external proposal including both UT and ORNL participation in order to be eligible for second-year funding. The Science Alliance plans to continue supporting StART projects with semiannual solicitations that provide more frequent opportunities for funding to faculty members.

This past fiscal year also saw the integration of graduate students into the Student Mentoring and Research Training Education (SMaRT) program. Despite the hurdles associated with research in the context of a global pandemic, the Science Alliance was able to continue supporting these graduate students in addition to facilitating a 10-week summer research experience for undergraduate SMaRT participants. The program will continue with a new class of undergraduate students in spring 2021.

The Graduate Advancement, Training and Education (GATE) program launched this year as well. GATE supports graduates students conducting meritorious collaborative research involving both the university and ORNL. Funding for the current class of GATE began August of 2020, and the Science Alliance plans to select the next cohort of GATE students at the beginning of 2021.

35 YEARS!

The Science Alliance celebrated its 35th anniversary of consistently funding UT-ORNL joint research in the fall of 2019.

Given the successful implementation of the first phase of the strategic plan, the Science Alliance intends to move forward with additional faculty development opportunities over the next year. While the StART program is aimed at nurturing new collaborations between faculty and ORNL researchers, many faculty members at the university have long-term robust collaborations with ORNL scientists. In an effort to support these ongoing relationships, the Science Alliance plans to implement a new Faculty Fellowship program. This program is designed to reward faculty by providing some of the benefits that are enjoyed by Distinguished Scientists through up to five fellowships.

The Science Alliance will also implement a program designed to develop research communities that will foster greater interactions between UT and ORNL and lead to increased meritorious research. The Partnership and Collaborative Teams (PACT) program will fund joint activities such as seminar series, poster sessions, and novel pilot projects for up to three years.

In order to ensure that the Science Alliance continues to provide opportunities and support in line with faculty needs, the first Science Alliance Advisory Board convened in June 2020 The advisory board will work to maintain open communication between the Science Alliance, faculty members, and ORNL staff; as well as serving as a reviewing body for new and ongoing commitments.

Over the next year, the Science Alliance will continue to provide support to faculty members engaging in meaningful collaborations with ORNL. Programmatic offerings will expand to reward high-performing faculty and develop research communities capable of pursuing large external awards. The Science Alliance will continue to integrate synergistically with the efforts of the newly established Oak Ridge Institute (ORI), further supporting innovation and developing opportunities for engagement in the local research community.

These initiatives will translate into global scientific and economic impacts, intellectual capacity development, and a prepared future workforce for Tennessee. Partnerships with and under the umbrella of ORI will aid both the university and ORNL in the development and acquisition of talented scientists and engineers, as well as continuing to provide consistent graduate student support in arenas of global interest.

DISTINGUISHED SCIENTISTS

The Science Alliance Distinguished Scientist Program supports high-profile joint leadership in research areas where UT and ORNL share complementary strengths. It has been the anchor program of the Science Alliance since 1984.

Distinguished Scientists hold tenured professorship at UT; most also hold a Distinguished Scientist appointment at ORNL, nominally half time at each institution. Appointments include an ongoing discretionary research fund equal to 12 months' salary.

Elbio Dagotto

Elbio Dagotto, a Distinguished Scientist in UT's Department of Physics and Astronomy and ORNL's Division of Materials Science and Technology, primarily uses computational techniques to study transition metal oxides, oxide interfaces, and the recently discovered iron-based high-temperature superconductors. These materials and others studied by his group show promise for both technological applications and advancing fundamental concepts in condensed matter physics.

Dagotto is the principal investigator of a fieldwork proposal at ORNL supported by the DOE's Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. This FWP has been active since 2007 and was recently renewed until 2021 with year-to-date funding of approximately $19 million. He is also the principal investigator of a subcontract from ORNL that provides support for three UT graduate students working on topics related to the DOE fieldwork proposal.

Takeshi Egami

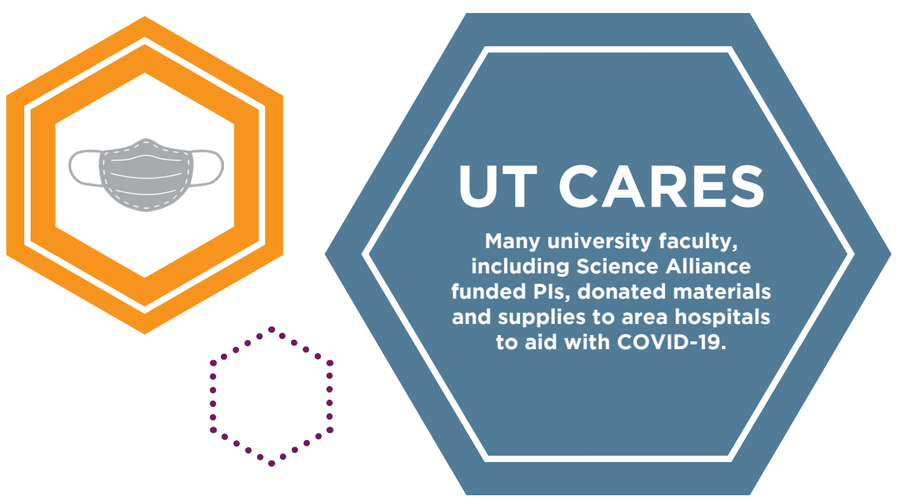
Takeshi Egami, Distinguished Professor in UT's Department of Materials Sciences and Engineering, explores new science involving liquids and gases. His work involves computer simulation (including quantum mechanical calculations) and neutron and synchrotron X-ray scattering experiments.

Egami is currently participating in a number of active collaborations with ORNL scientists, including DOE projects whose annual budgets total more than $2.7 million. His work has been repeatedly highlighted by the DOE in the past year.

Egami was recently named an Aris Phillips Lecturer, the most prestigious award given by the Department of Mechanical Engineering at Yale University. He serves as editor of Advances in Physics, a position he has held since 2011. In the past year he was named a Neutron Scattering Society of America Fellow.

EXTERNAL FUNDS

PRINCIPLE INVESTIGATOR	PROJECT TITLE	FY20 EXPENDITURES
DAGOTTO	Study of multi-orbital Hubbard models for iron-based superconductors and spin-orbit coupled transition metal oxides using the Density Matrix Renormalization Group technique	$50,990
EGAMI	Dynamics of Biologically Relevant Model Membrane Systems	$29,872
EGAMI	Neutron Scattering Study of Disordered Materials Under pressure	$34,091
EGAMI	Atomistic Studey of Bulk Metallic Glasses	$209,342
EGAMI	Fluid Interface Reactions, Structures and Transport (FIRST): Energy Frontier Research Center	$162,238
EGAMI	DMREF: Collaborative Research: Fundamentals of short-range order-assisted alloy design: Thermodynamics, kinetics, mechanics	$25,925



JOINT DIRECTED RESEARCH DEVELOPMENT

The Joint Directed Research Development (JDRD) program is one of the Science Alliance's longest-running initiatives. Historically the program provided funding opportunities for university faculty members working collaboratively with ORNL scientists supported by the Laboratory Directed Research Development (LDRD) program.

This year, the JDRD program was reformulated to take a narrowed approach, focusing on a list of research areas that facilitate the strategic goals of both the university and the lab. To ensure eligibility for as many faculty members as possible in light of the narrowed topic areas, the LDRD requirement was removed to allow collaborations with any relevant ORNL researcher.

JDRD awards continue to run for up to two calendar years. A progressive assessment at the end of year one determines if second-year funding will be awarded, based on partnership development and research progress.

Anahita Khojandi

Sepsis is estimated to kill around 250,000 Americans each year. In 2018, the state of Tennessee alone saw nearly 1,000 deaths as a result of sepsis. The JDRD work being done by Anahita Khojandi, associate professor of industrial and systems engineering, could lay the foundation for improving those outcomes.

Sepsis is a body's extreme reaction to an infection. This life-threatening condition typically occurs as a result of a pre-existing infection and has a mortality rate of around 40 percent. Survivability often depends on early identification and timely treatment of the condition. For every hour sepsis is undiagnosed, a patient's mortality rate increases by 8 percent. Patients in intensive care units, or ICUs, are especially at risk.

"It's actually one of the major causes of death in hospitals," said Khojandi. "It's very important to detect sepsis early, and because this is such an important problem we need to start addressing or thinking about it."

Khojandi's work seeks to improve sepsis outcomes by improving methods of early detection. Her team is working to combine Bayesian frameworks and machine learning to create a holistic means of peeking into the future of potential sepsis patients.

"For every minute a patient is in a nonsepsis state, there is a probability they will end up in sepsis. It's a very small probability, especially when you're looking at one minute, but then think about that over two or three hours. It's compounded," said Khojandi.

Khojandi believes the incorporation of a dynamic Bayesian framework will help account for the ongoing changes patients' bodies experience, allowing for a decrease in misdiagnoses. Such a holistic framework could also incorporate the human element, which could be especially relevant in ICUs.

"You have a limited number of nurses in ICUs caring for patients, so how should they prioritize based on risk factors? Who should they cautiously monitor, who should they closely attend to, who should they rank how in terms of these risk factors?" Khojandi asked.

Her JDRD team has partnered with hospitals to gain access to a data set for a pilot study. Additionally, they have generated several papers on the topic and submitted proposals to the National Science Foundation. Khojandi hopes this project will have multiple medical applications and improve outcomes for many people, both in and beyond Tennessee.

Michela Taufer

Neural networks—computational systems conceptually modeled after the brain—are an increasingly effective tool in modern data analysis. One challenge facing scientists using neural networks is the nature of their data.

Different types of data require the use of different neural networks. Michela Taufer, Dongarra Professor of High Performance Computing, hopes her JDRD project will make identifying the correct neural networks easier.

Humans have always found ways to complete tasks more quickly and effectively. Beginning around the 1980s, factories began to use more and more automation in order to generate products more quickly. The volume and pace of production outstripped human capability, so humans turned to computerized operation. Neural networks play a similar role in data analysis.

As more scientific data is generated through experimentation and computer modeling, the pace of processing that data in a timely fashion has created a need for computer systems capable of handling large amounts of information very quickly. However, neural networks are not a one-size-fits-all solution.

"The challenge is that different sciences have different data representation, and different experiments within a scientific domain have different types of data," said Taufer. "One neural network that identifies specific patterns may work well for one data set, but if you change or expand the data set, the neural network may fail."

Taufer's JDRD team is working to develop a framework for identifying the best neural networks for analyzing particular data sets, decreasing the amount of time a scientist has to spend looking for the best tool to use with their data.

"You can find the optimal network yourself and you can spend all your life looking for it. What we want is to have a trade-off between accuracy and time spent by using machine learning to identify some optimal networks," said Taufer.

Taufer is working in conjunction with Travis Johnston, research scientist in artificial intelligence for high performance computing at ORNL, to develop this framework for identifying neural networks. She hopes to expand her collaboration in the future to include colleagues at Japan's RIKEN Center for Computational Science. This project could also generate an enormous archive of annotated neural network data that could be used by the broader scientific community and artificial intelligence applications.

SUPPORT FOR AFFILIATED RESEARCH TEAMS

The Support for Affiliated Research Teams (StART) program provides funding for up to two years to faculty members exploring first and new collaborations with ORNL researchers. Funded proposals are eligible for second-year funding following a performance-based evaluation, including the preparation of an external proposal.

StART is the first Science Alliance program to offer two semiannual deadlines, in an effort to provide faculty members with greater flexibility and additional access to funding throughout the year. In its inaugural year, the StART program funded seven projects in areas ranging from machine learning in materials science to neuromorphic computing.

Mashid Ahmadi

Materials science has played an important role in the creation of many modern technologies, from lithium-ion batteries to improved steels. The development of new materials has led to innovation in a variety of fields, but the process can be lengthy and inefficient. Mashid Ahmadi, assistant professor of materials science and engineering, hopes to contribute to a better process.

“The historical approach to materials development has been random; basically they mixed a bit of one molecule and a little bit of another element and then examined the properties of this new material for suitable applications,” said Ahmadi.

For this StART project, Ahmadi’s team is working with materials for optoelectronic applications, such as solar cells. Solar power has become one of the most popular forms of alternative energy. By 2019, California had one million solar roofs in operation. However, solar cells have had limited efficiency in the past, ranging from around 13 percent to around 46 percent. In contrast, fossil fuels hover around 50 percent efficiency and hydroelectric energy can have efficiency rates as high as 90 percent.

Solar cells have also been expensive. Installation on a private residence has cost as much as $300,000 for cells with an average lifespan of 10 to 15 years. One reason is the high cost of materials used to create solar cells. Historically silicon has been a key component, but before it can be used it must be purified in an expensive process. The high cost and low efficiency of solar cells point toward a need for the development of new materials for building better cells.

Ahmadi’s StART project is using a combination of experimental techniques and machine learning to create a more effective means of determining which material compositions would be best for this application.

“We are basically exploring thousands of different possible compositions and trying to discover the best candidate for specific applications,” Ahmadi said. “For example, for a solar cell device, we need to find the material that has the highest optical absorption and is also stable.”

Ahmadi’s team managed to conduct much of the experimental portion of her work before closing her lab in keeping with university guidance regarding COVID-19. They were subsequently able to move forward with the machine learning component of the project while working remotely and engaging with their ORNL collaborator Maxim Ziatdinov, research scientist in computational sciences and engineering.

“Basically, the goal of this project is to develop a smarter way to discover materials, to predict what kind of materials will be needed for a particular application,” Ahmadi said.

Constance Bailey

On average, the US Food and Drug Administration approves 20 new drugs a year for public use. Each of those drugs has been on a decade-long journey of research and development that may have cost as much as $2.6 billion. The JDRD work of Constance Bailey, assistant professor of chemistry, could help reduce the time, and subsequently the costs, of drug development.

Creating pharmaceuticals is a complex process that typically begins in a lab. The process of constructing drugs relies heavily on understanding stereochemistry—how certain molecules exist in three-dimensional space.

"Stereochemistry is really important for developing safe pharmaceutical intermediates, the building blocks of complex molecules. If you can't control the stereochemistry, then the drugs don't fit together correctly," said Bailey.

Molecules have what Bailey describes as handedness. Putting two molecules together is similar to a handshake; one molecule acts as the right hand and one acts as the left hand, allowing them to fit together correctly. If both molecules are acting as the right hand, the handshake does not work correctly. Bailey's JDRD team is investigating how to control the handedness of particular molecules.

"Enzymes are really naturally good at doing this, so what we're trying to do is figure out how to selectively harness the enzymes in a fairly easy and trivial way to make one mirror image, or one hand into the other," said Bailey.

The ultimate goal of Bailey's work is to discover a method that will allow scientists to determine in advance what changes may be needed in a molecule in the context of an experiment. While the pharmaceutical industry may be one of the most immediately relevant areas that could benefit from Bailey's work, it is far from the only one.

"There are actually a lot of broad applications beyond just the pharmaceutical applications—for example, in materials. In a sense, the work we're doing is kind of a fundamental science problem," said Bailey. "How do you selectively create three-dimensional structures that could have applications in all different areas of chemistry?"

Bailey's team adapted to the university-wide changes due to COVID-19 by having online meetings with their collaborator, Omar Demerdash, Liane B. Russell Distinguished Fellow in the Biosciences Division at ORNL. While her lab was closed, Bailey and her students used their time to dig deep into the literature and formulate an updated strategy for moving forward.

Francisco Barrera

Neuromorphic computing, which uses the human brain as design inspiration for computer systems, has been steadily gaining interest since the 1980s. Its potential to improve both speed and energy efficiency in computing, and subsequently supercomputing, make neuromorphic computing a thriving area of interest.

While not attempting to directly copy the human brain, neuromorphic computing draws inspiration from neurons and synapses to develop new means of computation and information transfer. Innovation is an important part of the field, and Francisco Barrera, associate professor of biochemistry and cellular and molecular biology, is bringing a new approach to chip development.

Historically Barrera's work has focused on the plasma membrane—a protective barrier between individual cells and their external environments that also regulates communication between cells. For this StART project, Barrera is working in collaboration with Pat Collier, a staff researcher at ORNL.

"The Collier laboratory is working to recreate how neurons work using a system called droplet interface bilayer," said Barrera. A droplet interface bilayer, or DIB, system includes small membranes that closely mimic the plasma membrane of neurons. When connected, these membranes have been shown to do some promising computing.

Barrera's team is working to improve the function and connectivity of these membranes. They have designed a peptide that, when added into the membranes, can change how currents move across them, which is important for communication.

"What I think is very exciting is that I believe we can make an important contribution because we try to understand, at a very deep level, how our peptides interact with lipids in the membrane," said Barrera. "This is the kind of basic knowledge that allows you to understand a system and predict how it will respond."

Barrera hopes the discoveries made with this StART project will ultimately lead to increased power and flexibility in chips for neuromorphic computing.

Sindhu Jagadamma

Carbon is the foundation of all life on Earth and a central component of climate, food production, and energy creation. Carbon cycling is the way carbon is recycled or moved around from the atmosphere into organisms and soil and back out again. Changes to any component of the process have the ability to impact the carbon cycle, but the potential effects of soil composition are not well understood. Assistant Professor of Biosystems Engineering and Soil Science Sindhu Jagadamma hopes to improve that understanding.

Plants pull carbon dioxide from the air and, through photosynthesis, convert it to plant biomass, which ultimately ends up in soil as soil carbon. Soil carbon is critical to sustainable food production, playing a vital role in soil, water, and air quality. Securely storing carbon in soil is also important for reducing the concentration of carbon dioxide in the atmosphere.

Soil composition plays an important role in soil carbon cycling. For example, manganese content in soil can impact carbon cycling by influencing photosynthesis and litter decomposition. Jagadamma's StART project is focusing on the impact of manganese on the balance of carbon within agricultural soil systems.

"It is really important to understand the different drivers of carbon cycling in soil in order to build healthy soils and promote sustainability," said Jagadamma. "The role of manganese in influencing carbon decomposition is relatively unknown, especially in agricultural soils."

Jagadamma points out that nitrogen fertilizers may create more acidic soil, which increases manganese availability. While manganese is an essential nutrient for plants, excess manganese in soil can inhibit plant growth and lead to lower crop yields. However, a comprehensive study determining the link between manganese, carbon cycling, and the impact on croplands has yet to be completed.

Jagadamma's ORNL collaborator, Staff Scientist in Environmental Sciences Elizabeth Herndon, has begun this work with laboratory and field experiments in forested ecosystems. The knowledge generated by these experiments is being used by Jagadamma's team to extend the research into the agricultural field.

"We are going to manipulate different levels of manganese in soil, grow plants, and see if the different levels of manganese are influencing plant growth and litter decomposition, and how it is ultimately going to influence the carbon cycle," said Jagadamma.

Her project, like so many others this year, was delayed due to COVID-19 precautions, but she hopes to move into the experimental phase next spring. In the meantime, she and her team have focused on literature review and a lab-scale pilot study to assist in developing the most meaningful field experiment for the spring.

Jagadamma's StART project will have obvious implications for agriculture. If soil manganese is altered by nitrogen fertilization and other human-induced changes, and if those altered manganese levels change soil carbon storage, cropland systems can be developed for better crop growth and carbon storage. This work will also have broad implications for global carbon cycling by helping find ways to curb carbon dioxide levels in the atmosphere.

Hugh Medal

The Materials Genome Initiative, or MGI, was announced in 2011 as a multiagency initiative to increase the speed of advanced materials development and production. Since then the federal government has invested more than $250 million in new research and innovation infrastructure to help achieve that goal. Assistant Professor of Industrial and Systems Engineering Hugh Medal hopes his StART project will contribute to the work of the MGI.

A key MGI program, the Materials Project, has amassed a database of hundreds of thousands of materials with their predicted properties—information that would normally require repeated experimentation to discover. Knowing that the materials can exist, however, is not the same thing as successfully creating them. While the simulations contributed to the Materials Project may point toward potential new materials, figuring out how best to produce those materials is left to experimentation.

"Making a material is a lot more complicated than just putting components together," said Medal. "Think about steel. It's not just a matter of adding different elements from the periodic table. It requires applying a lot of different processing actions in order to get the material to its final state, or phase."

The question of how best to develop these predicted materials is a large one in materials science. Medal is attempting to make inroads in this area with his StART project. His team is collaborating with Haixuan Xu, associate professor of materials science and engineering and a former Science Alliance JDRD awardee, to create a simulation that can predict how to produce these materials.

"We're working together to come up with a technique that can tell us how—given a predicted material that's really interesting, what processing do we need to apply over time to be able to grow that material," said Medal.

Leveraging Xu's expertise in modeling the kinetic behavior of materials and Medal's work with machine learning, the team hopes to develop a tool to serve as a guide for those working toward creating predicted materials.

"Our hope is that our tool that will simplify the process. Rather than having experimentalists sift through a large number of combinations of processing actions, we want our tool to point toward the processes that would most likely be successful," said Medal.

Zhenbo Wang

In 2009 the Google Self-Driving Car Project made its debut, ushering in an age of interest and research in automated vehicles. Connected and automated vehicles, or CAVs, have continued to capture the attention of researchers who are attempting to address some of the fundamental problems with connective vehicle technology. Zhenbo Wang, assistant professor of mechanical, aerospace, and biomedical engineering is tackling one of these problems: intersections.

CAVs use a variety of technologies to communicate with other connected devices around them, including other cars, roadside assistance services, and even traffic signals. These communications could potentially help drivers and vehicles make adjustments to improve efficiency, such as decelerating for an approaching intersection.

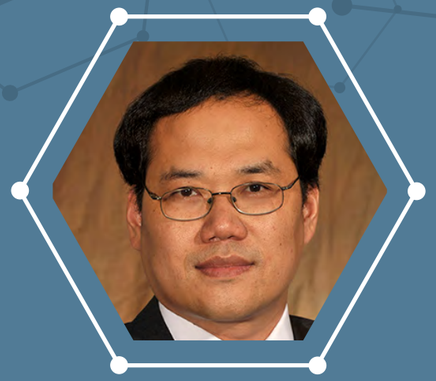
"What I'm doing with this project is trying to better control ground vehicles based on traffic signal changes," said Wang. "The traffic signal will broadcast information to oncoming vehicles, and we want to know how we can optimize the motion of the vehicle to, for example, minimize fuel consumption."

In addition to improved fuel efficiency, CAVs have major implications for road safety. According to the Tennessee Department of Safety and Homeland Security, there were more than 1,100 traffic fatalities in the state last year. Among the primary causes of these accidents are distracted driving, driving under the influence, and speeding—in other words, human error. CAVs may be able to decrease fatal traffic accidents by using connections with other devices to reduce risk, such as communicating to oncoming vehicles that a car is about to run a red light.

Wang's StART team hopes to develop a control strategy for vehicles using traffic signal phase and timing data to make real-time speed adjustments in response to information received. These adjustments will contribute to better fuel efficiency and a host of other benefits.

Wang is working in collaboration with Tim LaClair, research and development engineer at ORNL, whose team has developed expertise in modeling, simulation, and control of CAVs. Their long-term goal is to develop a framework for controlling CAVs that works effectively with the large amounts of data generated by the traffic network.

"Connected vehicles have the potential to revolutionize transportation," said Wang. "To realize that potential we need to develop algorithms to control these vehicles in real time to reduce congestion, maximize fuel economy, and increase safety."



Xiaopeng Zhao

Alzheimer's disease is responsible for between 60 and 80 percent of dementia cases. A progressive disease that attacks the human brain, Alzheimer's produces symptoms that include memory loss, difficulty thinking, and behavioral changes that can worsen over time. More than five million Americans are living with Alzheimer's, a number projected to reach 16 million by 2050.

While no cure for Alzheimer's exists, researchers have begun to consider the possibility of treatment with devices using brain-computer interfaces, or BCIs. Xiaopeng Zhao, professor of mechanical, aerospace, and biomedical engineering, hopes to contribute to the body of research that could make development of such treatments possible.

Brain-computer interfaces—sometimes called mind-machine interfaces—essentially create a direct line of communication between the brain and an external device. BCIs are being investigated for uses in mapping, assisting, and even repairing cognitive, sensory, and motor functions. For these potential therapies to be effective, interfaces need further development.

Repeated hospital admission is one hurdle facing Alzheimer's and other dementia patients. A number of factors contribute to hospital readmissions, but there is evidence that appropriate care plans and therapies may help reduce these. This is where Zhao's work with BCIs could play an important role.

Zhao has historically worked on developing cognitive training for Alzheimer's patients and has also developed BCI systems for a variety of applications, including robotic arms, drones, and wheelchairs. In this StART collaboration with Zhiming Gao in ORNL's Fuel, Engines and Emission Research laboratory, Zhao's team is developing a BCI for use in connected vehicle technology. He hopes this work will eventually be applicable in a medical context.

"We want to understand human memory and attention in general—so basically the executive function," said Zhao. "We're working on the human side, so we look at how humans experience driving or riding. Can we detect the intention or emotion of that person and use it to improve the experience?"

Zhao acknowledges that while Alzheimer's and driving may seem to be unrelated, the BCI advances made to develop connected driving can serve to improve interfaces used for medical purposes. He hopes to eventually build a gamified driving simulator to monitor and evaluate cognitive behaviors.

"Do they experience attention deficits? Do they have short-term memory loss? Can we use driving as a means of evaluating these problems?" asked Zhao. "Eventually I believe this will connect to my other research line in working with Alzheimer's."

STUDENT SUPPORT

In an effort to deepen the Science Alliance's existing commitment to student support, this year saw the implementation of a new program for undergraduate and graduate students. The Student Mentoring and Research Training (SMaRT) program provides opportunities for undergraduate students to engage in a year-long mentored research experience that includes an intensive 10-week summer research internship performing a collaborative project with UT and ORNL faculty and staff.

Beginning in spring, participating undergraduates are mentored by graduate students supported by the program. Graduate mentors prepare the undergraduate students for the summer and help with dissemination of the work afterward. Presented in partnership with the Tennessee Louis Stokes Alliance for Minority Participation and UT's Student Support Services and Office of Undergraduate Research, the SMaRT program provides hands-on experience to undergraduate students in a national laboratory setting.

In its inaugural year, the program had to undergo a rapid reformulation in order to comply with COVID-19-related restrictions at both the university and ORNL. Keeping student safety at the forefront, faculty mentors pivoted to provide remote work opportunities for as many students as possible. Labs continuing to operate in person implemented stringent safety procedures to ensure the health and well-being of faculty members and students.

Despite these challenges, the overwhelming majority of SMaRT students participated in Discover Day, a research event sponsored by the Office of Undergraduate Research. Students presented posters describing the projects in which they had participated over the summer. Those who were comfortable doing so were able to present in person, and an online participation option allowed students to submit a digital poster and upload a brief video of their presentation.

GRADUATE STUDENT SUPPORT

Integral to the charter of the Science Alliance is this principle: Science Alliance funding will be used to "provide incentives to attract and retain the highest quality students and strengthen the educational opportunities for both UT and ORNL." Consequently, each year a portion of the Science Alliance's funding is distributed directly to two colleges within the university with the express purpose of supporting graduate education and research. As a result, many students have had occasion to add significantly to the foundation of their careers through direct support provided by Science Alliance.

Here are some of the past year's graduate student research highlights:

Yang Shi, a graduate student working with Zhenbo Wang, is working on advanced control, optimization, and machine learning techniques for connected vehicles. His research interests center on data-driven approaches for traffic signal control, and he is currently working with traffic signal phase and timing data.

Mashid Ahmadi's StART project supports multiple graduate students. **Amanda Heimbrook** has gained experimental and coding skills. For her research, she has learned to use an automated robot to eliminate human error from samples. **Kate Higgins** has worked with Ahmadi to develop a workflow for automated synthesis and characterization of materials using a robot.

Jeremy Watts is working on a JDRD team with Anahita Khojandi. He has co-authored a publication on his work developing realistic patient environment models as a means of developing more effective treatment plans for patients with Parkinson's disease.

Science Alliance–funded graduate student **Fengpie Yuan** is also working to address disease. His research is focused on cognitive training and socially assistive robots, which could have applications for Alzheimer's disease. Yuan is helping Xiaopeng Zhao's StART team develop a brain–computer interface for monitoring a user's neurophysical status during driving tasks.

Nolan Spengler is a second-year graduate student working with Constance Bailey. His work has focused on developing analytical methods of testing the stereospecificity, or handedness, of enzymes. This work contributes directly to Bailey's StART project.

Many Science Alliance–funded graduate students are actively collaborating with ORNL scientists. They have earned additional funding for their work from a variety of sources, including the National Science Foundation, the US Department of Energy, and NASA. Many also serve as mentors to the undergraduate students on their teams. The contributions made by these scholars not only prepare them for future careers but also help ensure a significant presence foothold for the University of Tennessee and the state in the future of the nation's scientific community.

GRADUATE STUDENT SUPPORT BY DEPARTMENT

DEPARTMENT	TOTAL SUPPORT	# OF STUDENTS	HIGHLIGHTS
BIOLOGY	$302,270	33	Integral to the charter of the Science Alliance is this principle: Science Alliance funding will be used to "provide incentives to attract and retain the highest quality students and strengthen the educational opportunities for both UT and ORNL." Consequently, each year a portion of the Science Alliance's funding is distributed directly to two colleges within the university with the express purpose of supporting graduate education and research. As a result, many students have had occasion to add significantly to the foundation of their careers through direct support provided by Science Alliance.
CHEMISTRY	$156,119	17	Chemistry students supported by Science Alliance had multiple ORNL and governmental affiliations, including with DOE, NSF, and NIH. They co-authored more than 20 publications and one student received the Excellence in Polymer Graduate Research award at the American Chemical Society national meeting. Another student has contributed to a provisional patent.
EARTH & PLANETARY SCIENCES	$37,548	6	Funded students co-authored two publications and five of the sixe students made a total of 12 meeting or conference presentations. All students have external affiliations or funding sources including ORNL, DOE, NASA, and the U.S. Army.
ELECTRICAL ENGINEERING & COMPUTER SCIENCES	$108,588	11	Supported students maintained both governmental affiliations, such as DOD, NSF and USDA, and industry affiliations with Mercedes Benz and Cree Fayetville Inc. These students co-authored three publications and presented at two conferences. One student was a recipient of a Tennessee Top 100 Graduate Fellowship.
MATHEMATICS	$97,795	18	All funded mathematics students engaged in an ORNL affiliation. This group of students helped generate five publications and six conference or meeting presentations.
PHYSICS	$222,500	26	Supported students co-authored nine publications and made 14 conference or meeting presentations. Almost 90% of students maintained a relationship with ORNL. As a result of ongoing work with the Center for Materials Processing, one student has a research record of 39 total publications. One student received the NSF Nanoscholar II scholarship. Another student organized a 10 week summer fellowship program for undergraduate students.
PSYCHOLOGY	$10,022	1	The single supported student co-authored three publications and was awarded a Chancellor's Fellowship and the Chancellor's Citation for Extraordinary Professional Promise.

SMaRT PROGRAM

Aruha Khan, working with Lawrence Heilbronn, John D. Tickle Professor of Nuclear Engineering, studied targeted alpha therapy, specifically for prostate cancer treatment. Khan completed a cross-sectional analysis of laboratory and clinical results to show that targeted alpha therapy can provide a therapeutic option to patients who are resistant to traditional treatments.

Biochemistry and cellular and molecular biology student **Alice Huang** worked in conjunction with Bob Hettich, Distinguished Research Scientist in the Mass Spectometry/Laser Spectroscopy Group at ORNL, on a National Science Foundation–funded exploration of proteins of unknown functions. Huang leveraged bioinformatics tools, public databases, and existing protein and DNA sequence analyses for this work.

Zachy Hussein worked with Chad Duty, associate professor of mechanical, aerospace, and biomedical engineering. As part of his summer work experience, Hussein worked on a study to determine if polymer feedstocks could be used in a common desktop 3D printer. For this exploration he developed proficiency with a Lulzbot 6 3D printer.

Working together, **Mya Pinson** and **Elexis Allen** focused on plant genome sequencing. Under the guidance of Anahita Khojandi, associate professor of industrial and systems engineering and current Science Alliance StART awardee, Pinson and Allen gained a number of skills, including working with the Oxford Nanopore Technologies MinION sequencing device and application of the Basic Local Alignment Search Tool (BLAST) algorithm.

Nuclear engineering student **Jay Artley** worked with fourth-generation nuclear reactor technology focusing on molten salt reactors. For this work, he helped develop models of molten salt reactors and compared their output to the results of the Molten Salt Reactor Experiment (MSRE) conducted by ORNL in the 1960s.

DID YOU KNOW?

More than 85% of SMaRT undergraduate students presented their work, either virtually or in-person, at Discover Day 2020.

UNDERGRADUATE STUDENT SUPPORT BY DEPARTMENT

DEPARTMENT	TOTAL SUPPORT	# OF STUDENTS
BIOCHEMISTRY AND CELLULAR AND MOLECULAR BIOLOGY	$12,175	2
CHEMISTRY	$13,097	3
ELECTRICAL ENGINEERING & COMPUTER SCIENCES	$24,622	4
INDUSTRIAL & SYSTEMS ENGINEERING	$18,102	3
MATERIAL SCIENCE ENGINEERING	$7,841	2
MECHANICAL AEROSPACE AND BIOMEDICAL ENGINEERING	$24,207	4
NUCLEAR ENGINEERING	$42,394	7
PHYSICS	$12,028	2

UT-ORNL JOINT INSTITUTES

UT-ORNL Joint Institute for Advanced Materials
The Joint Institute for Advanced Materials promotes interdisciplinary research and education related to developing new materials with superior properties, such as greater toughness and high-temperature strength, or those that can be tailored to support new technologies, such as pocket-sized supercomputers.

UT-ORNL Joint Institute for Biological Sciences
The Joint Institute for Biological Sciences supports interdisciplinary, crosscutting research that accelerates progress in complex bioenergy and bioenvironmental systems. It also aids access by UT-ORNL faculty, staff and students to state-of-the-art capability in genomic, transcriptomic, proteomic, and metabolomic analysis of biological and environmental systems.

UT-ORNL Joint Institute for Computational Sciences
The Joint Institute for Computations Sciences (JICS) advances scientific discovery and state-of-the-art engineering and computational modeling and simulation. JICS takes full advantage of the petascale and beyond computers in the DOE National Center for Computations Sciences and UT's National Institute for Computational Sciences.

UT-ORNL Joint Institute for Nuclear Physics and Applications
The Joint Institute of Nuclear Physics and Applications links UT, ORNL and Vanderbilt University research to promote and support basic nuclear physics research and nuclear and radiological applications of common interest to the participants.

UR-ORNL Shull Wollan Center, a Joint Institute for Neutron Sciences
The Shull Wollan Center promotes worldwide neutron scattering collaboration among researchers in biological and life sciences, energy sciences, polymer science, condensed matter physics, and computational sciences.

PUBLICATIONS

Elbio Dagotto

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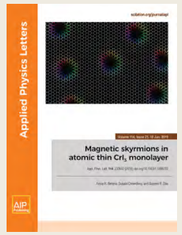

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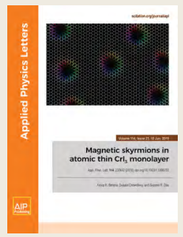
Anahite Khojandi



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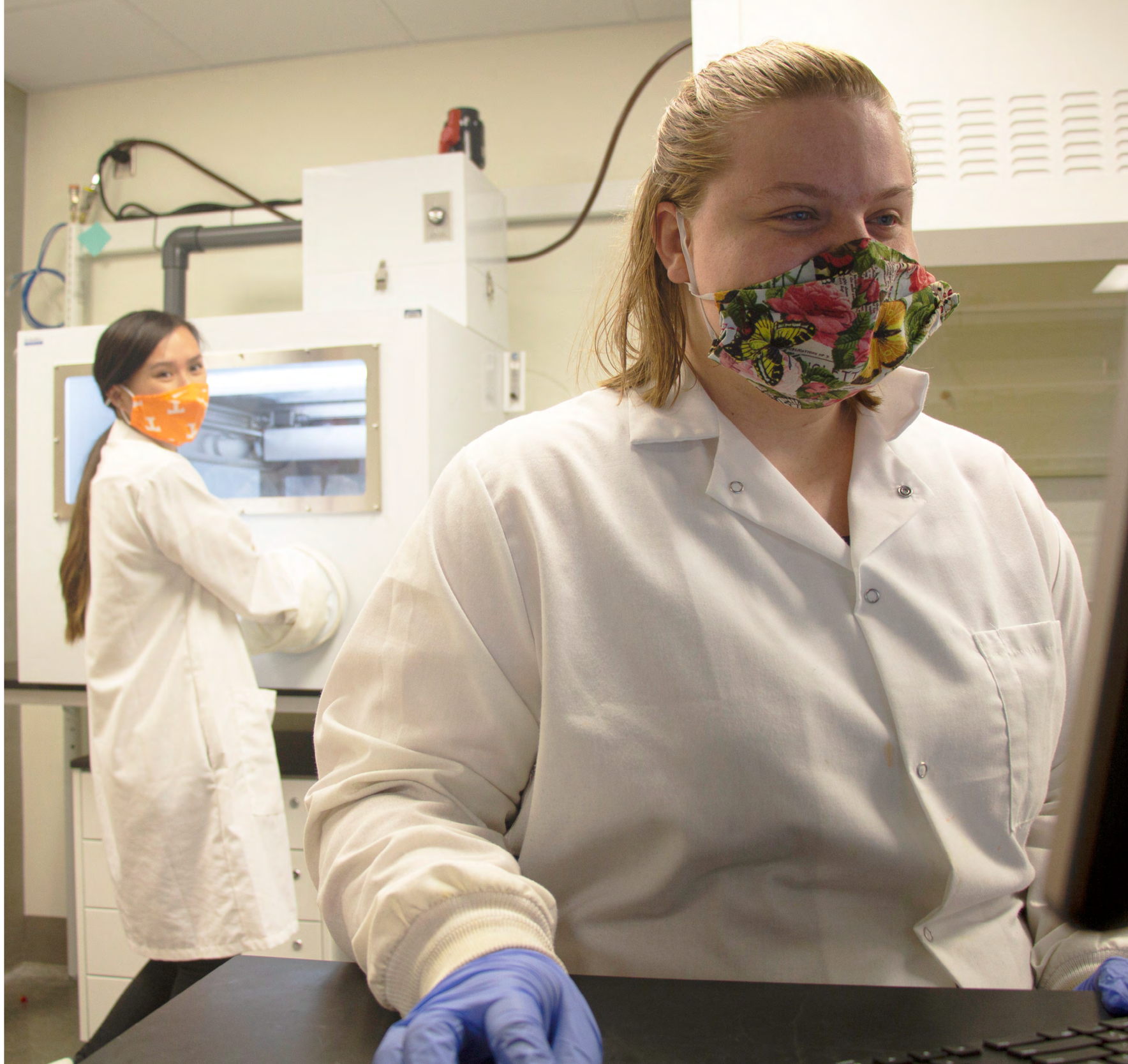
60+ AND COUNTING!

Science Alliance funded graduate students developed more than 60 conference presentations or publications.



Schedule 7

CENTERS OF EXCELLENCE ACTUAL, PROPOSED, AND REQUESTED BUDGET

Institution: The University of Tennessee

Center: The Science Alliance

	FY 2019-20 Actual			FY 2020-21 Proposed			FY 2020-21 Requested		
	Matching	Appropr.	Total	Matching	Appropr.	Total	Matching	Appropr.	Total
Expenditures									
Salaries									
Faculty	$459,611	$447,709	**$907,320**	$473,399	$850,000	**$1,323,399**	$497,069	$892,500	**$1,389,569**
Other Professional	217,366	198,338	**415,704**	$223,887	$204,288	**428,175**	$235,081	$214,503	**449,584**
Clerical/ Supporting	81,777	271,070	**352,846**	$84,230	$279,202	**363,432**	$88,442	$293,162	**381,603**
Assistantships	127,115	1,217,103	**1,344,217**	$130,928	$1,941,396	**2,072,324**	$137,475	$2,038,466	**2,175,940**
Total Salaries	**$885,868**	**$2,134,219**	**$3,020,088**	**$912,444**	**$3,274,886**	**$4,187,330**	**$958,067**	**$3,438,630**	**$4,396,697**
Longevity (Exclude from Salaries)	$6,350	$2,708	**$9,058**	$6,541	$2,789	**$9,330**	$6,868	$2,929	**$9,796**
Fringe Benefits	$227,688	297,769	**525,457**	$234,519	$306,702	**541,221**	246,245	322,037	**568,282**
Total Personnel	**$1,119,907**	**$2,434,696**	**$3,554,603**	**$1,153,504**	**$3,584,377**	**$4,737,881**	**$1,211,179**	**$3,763,596**	**$4,974,775**
Non-Personnel									
Travel	$30,020	$47,719	**$77,740**	$75,000	$150,000	**$225,000**	$31,521	$40,000	**$71,521**
Software	220	2,600	**2,820**	2,500	5,000	**7,500**	231	2,730	**2,961**
Books & Journals	2,123	910	**3,033**	7,500	15,000	**22,500**	2,229	956	**3,185**
Other Supplies	15,957	94,491	**110,449**	200,000	300,069	**500,069**	16,755	95,000	**111,755**
Equipment	6,706	6,706	**13,411**	240,000	480,000	**720,000**	100,000	10,000	**110,000**
Other (Specify):									
Prof Services & Memberships	$21,897	$179,560	**$201,456**	125,000	250,000	**375,000**	22,991	50,000	**$72,991**
Motor Vehicle Operations		1,795	**1,795**	2,500	5,000	**7,500**	-	1,884	**1,884**
Printing, Duplicating, Binding	42	57	**99**	2,500	5,000	**7,500**	44	60	**104**
Communications	1,094	840	**1,935**	2,500	5,000	**7,500**	1,149	882	**2,031**
Computer Services	696	348	**1,044**	225,000	450,000	**675,000**	731	365	**1,096**
Grants and Subsidies (Student Fees)	458,107	176,362	**634,469**	1,100,000	1,087,900	**2,187,900**	592,723	57,000	**649,723**
Contractual & Special Services	58,764	67,803	**126,567**	200,000	400,000	**600,000**	61,702	71,108	**132,810**
Utilities & Fuel		269	**269**	500	1,000	**1,500**	-	282	**282**
Insurance, Interest & Bad Debt	6,277	7,244	**13,521**	5,000	10,000	**15,000**	6,591	7,606	**14,197**
Other Expenditures	4,240	2,979	**7,219**	35,000	70,000	**105,000**	4,452	3,128	**7,580**
Cost Sharing		57,495	**57,495**	1,451,964	2,838,591	**4,290,555**	-		**-**
Total Non-Personnel	**$606,143**	**$647,178**	**$1,253,321**	**$3,674,964**	**$6,072,560**	**$9,747,524**	**$841,120**	**$341,002**	**$1,182,121**
GRAND TOTAL	**$1,726,050**	**$3,081,873**	**$4,807,924**	**$4,828,468**	**$9,656,937**	**$14,485,404**	**$2,052,299**	**$4,104,597**	**$6,156,896**
Revenue									
New State Appropriation		$3,901,568	**$3,901,568**		$3,909,140	**$3,909,140**		$4,104,597	**$4,104,597**
Carryover State Appropriation		4,928,102	**4,928,102**		$5,747,797	**5,747,797**			**-**
New Matching Funds	1,726,050		**1,726,050**	4,828,468		**4,828,468**	2,052,299		**2,052,299**
Carryover from Previous Matching Funds			**-**			**-**			**-**
Total Revenue	**$1,726,050**	**$8,829,670**	**$10,555,720**	**$4,828,468**	**$9,656,937**	**$14,485,404**	**$2,052,299**	**$4,104,597**	**$6,156,896**

THE UNIVERSITY OF TENNESSEE KNOXVILLE

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