

SCIENCE ALLIANCE

**Annual
Report
2021-2022**

*THEC State
Appropriations
Request 2023-2024*



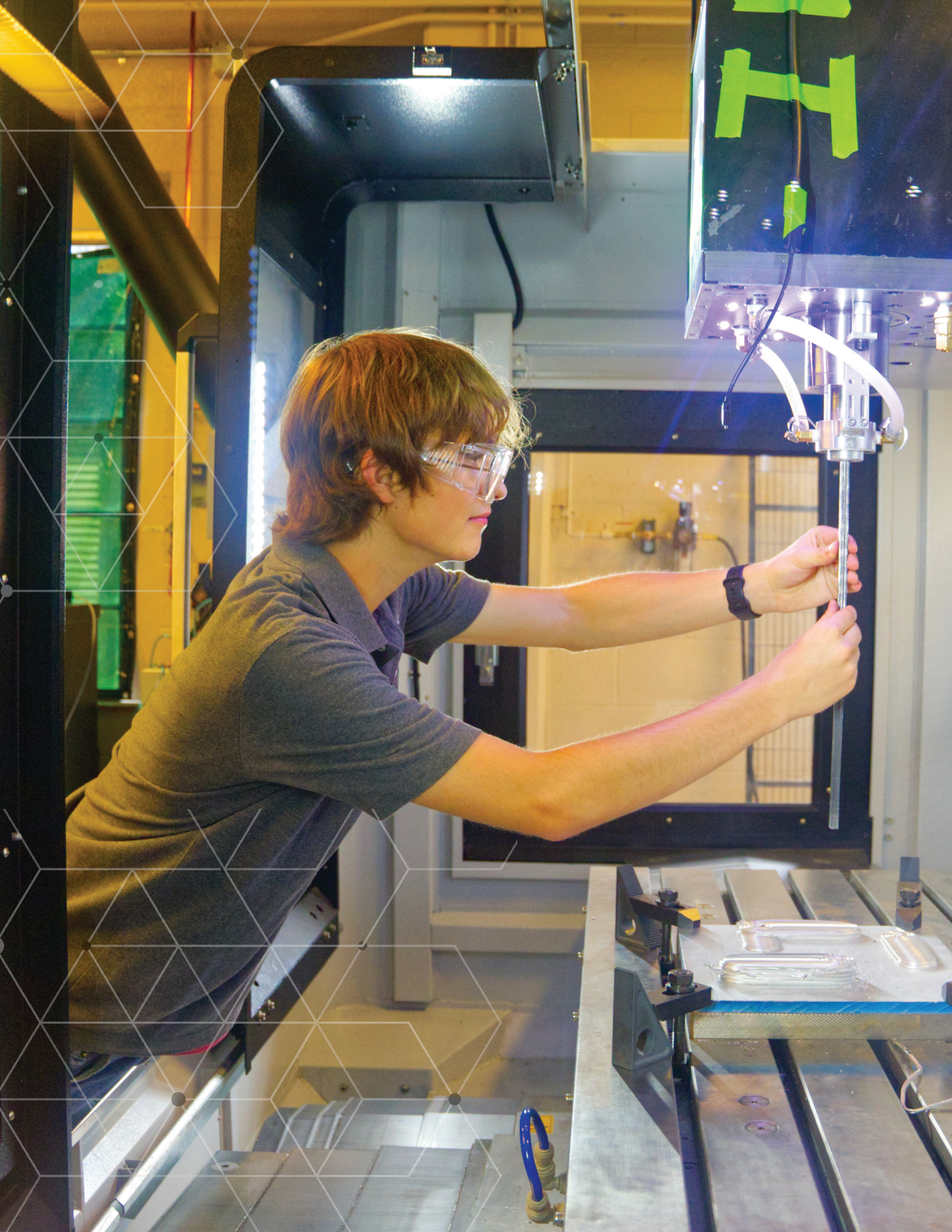


Table of CONTENTS

Executive Summary & Science Alliance Overview	04
Mission Statement, Goals & Future Plans	06
Distinguished Scientists	09
Joint Directed Research Development (JDRD)	11
Support for Affiliated Research Teams (StART) Awardees	15
Program for Advancing Collaborative Teams (PACT) Awardee	21
Student Support	22
Graduate Advancement, Training & Education (GATE) Awardees	24
Student Mentoring and Research Training (SMaRT)	30
Undergraduate Support	32
Publications	33

Executive Summary

The Science Alliance is the longest continually operating organization facilitating collaborations between the University of Tennessee, Knoxville and Oak Ridge National Laboratory (ORNL). Having successfully navigated the pandemic, the past year has brought a return to normalcy, including invaluable face-to-face interactions between collaborating faculty, staff, and students.



Shawn Campagna

*Faculty Fellow for Research Development
Director of Scientific Programs & Science Alliance*

As we wrap up one fiscal year and embark on another, we stand on a strong history and step enthusiastically into a future filled with possibilities.

For the past several years, we've been re-envisioning Science Alliance and implementing new programs. With the Science Alliance now fully integrated into the University of Tennessee-Oak Ridge Innovation Institute (UT-ORII), we're looking at our next phase of growth: Redefining existing programs and unveiling new programs to further enhance the greater research enterprise.

The Science Alliance prioritizes relationships between UT and ORNL faculty and researchers. Many of our programs, such as the Support for Affiliated Research Teams (StART) program, focus on building those relationships early in a faculty member's career at UT. Science Alliance provides UT faculty members with up to two years of support to explore first and new collaborations with ORNL researchers to develop proof of concept for new ideas that can expand into novel research paths.

At the same time, the Science Alliance also values relationships with long-term faculty members who have already developed robust collaborations with ORNL partners. This past year, we launched our Faculty Fellows program to support the work of some of these UT researchers. We've also continued to grow the Partnership and Collaborative Teams (PACT) program which began in fiscal year 2020-21 to nurture greater interactions between UT and ORNL and promote meritorious research.

Building on the momentum of past years, we've expanded the Student Mentoring and Research Training (SMaRT) program. A cohort of 42 students from 31 universities across the country converged on UT's campus over the summer to engage in cutting-edge research while being supported by graduate students and high-performing faculty mentors. Our goal, of course, is to recruit the top students from this group back to UT for their graduate studies and to build their careers in Tennessee.

The Science Alliance's student support strategy continued to provide extensive graduate student support via direct funding to departments across campus, as well as through individual student awards through the Graduate Advancement, Training, and Education (GATE) program. Together, these two programs represent an investment of more than \$1.3 million in the future of research in Tennessee and beyond.

This report illustrates the synergy of faculty and students who are committed to exploring big and important ideas. In this report, we share success stories, budding collaborations, and academic achievements. Science Alliance awards continue to invest in the university and its people, building a competitive future for the state of Tennessee.

A smiling man with a beard and safety glasses is shown in profile, working in a laboratory. He is wearing a dark blue polo shirt with "MT" visible on the sleeve. The background shows various laboratory equipment and a bright orange safety barrier.

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 materials, clean manufacturing and materials science; energy storage; transportation; 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.



Science Alliance MISSION

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 opportunities
- 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 & Future Plans

Since its inception, the Science Alliance's mission has been to create opportunities for meaningful collaborations between the University of Tennessee, Knoxville and Oak Ridge National Laboratory (ORNL).

In the past year, the Science Alliance integrated into the UT-Oak Ridge Innovation Institute (UT-ORII), expanded existing programs, and introduced a new one.

The Support for Affiliated Research Teams (StART) program, launched in the 2019-2020 fiscal year, provides UT faculty members with up to two years of support to explore first and new collaborations with ORNL researchers. Researchers qualify for the second year of funding when they produce an external proposal that includes the participation of both ORNL and UT. Total new funding awarded during the past fiscal year for StART totaled \$493,000, with three faculty members receiving first-year funding and three receiving funding for all or part of a second year. Collectively, those faculty are working with six undergraduates, 11 graduate students, and two post-docs. The Science Alliance plans to continue supporting StART projects with semi-annual solicitations that provide more frequent opportunities for funding to faculty members.

The Joint Directed Research Development (JDRD) program, a dual UT and ORNL venture that has facilitated collaboration between researchers from both institutions for a decade, provided \$249,549 in second-year funding to three faculty members who collectively worked with two undergraduates, 10 graduates, two post-docs, and three research associates. The JDRD program is being reconceptualized to create greater cohesion around topics of mutual strategic interest for both institutions.

This past year also saw growth in the Student Mentoring and Research Training Education (SMaRT) program, which began in fiscal year 2019-2020. SMaRT seeks to promote research and utilize the unique partnership between UT

and ORNL by funding paid undergraduate internships that focus on ORNL-related research with a UT faculty member. Our ultimate goal with the program is to recruit our top students to UT for grad school and to build their careers in Tennessee.

The Science Alliance worked in conjunction with Oak Ridge Associated University (ORAU) to recruit 41 exemplary undergraduate students from across the country to work with 10 UT faculty members during the summer of 2022. Students were housed on campus for 10 weeks while they engaged in research and professional development opportunities. The program culminated in a research symposium where students delivered formal presentations and posters to an audience of their peers, faculty members, and administrators. To date, SMaRT program funding has been about \$835,000.

In addition to the support provided to students via the SMaRT program, the Graduate Advancement, Training, and Education (GATE) program continued to provide funding to graduate students conducting meritorious, collaborative research through the 2021-2022 academic year. In its first two years, from August 2020 to June 2022, the program involved 25 students and provided them with funding totaling \$1,640,239. The next cohort of GATE students was selected at the end of that academic year and began receiving funding on August 1, 2022. The GATE program operates alongside historical funding the Science Alliance provides to many departments across campus for graduate student support; both efforts help develop future research professionals.

The Partnership and Collaborative Teams (PACT) program, which started in February 2022, is designed to develop research communities that will foster greater interactions between UT and ORNL and lead to increased meritorious research. To date, PACT funding has totaled \$198,166.





Goals & Future Plans Continued

This past year, the Science Alliance also launched its Faculty Fellows program. While the StART program is aimed at nurturing new collaborations between faculty and ORNL researchers, many UT faculty members have long-term, robust relationships with ORNL scientists. To support these ongoing collaborations, the StART program is designed to reward UT faculty by providing some of the benefits that are enjoyed by distinguished scientists through up to five fellowships. The first 10 fellows, each awarded \$8,000 plus benefits for a total of \$94,673.14, are: Associate Professor Scott Emrich, Professor Gong Gu, Professor Jian Huang, Professor Michael Langston, Assistant Professor Jian Liu, and Professor Kai Sun, all from the Min Kao Department of electrical engineering and computer science; Professor Xiaopeng Zhao, from the Department of Mechanical, Aerospace and Biomedical Engineering; Professor Paul Armsworth, of the Department of Ecology and Evolutionary Biology; Assistant Professor Hugh Medal, from the Department of Industrial and Systems Engineering; and Assistant Professor Constance Bailey from the Department of Chemistry.

As we look to the future, the Science Alliance will work under the umbrella of UT-ORII to promote professional

relationships between the UT and ORNL research communities to inspire creative synergy and meaningful collaborations that advance groundbreaking science, and impact the state of Tennessee and the global economy.

Science Alliance programs will continue to reward high-performing faculty, support early-career faculty, and encourage students who will blaze future trails of research. The Science Alliance will also support efforts, such as the UT-ORII seed program, that develop multidisciplinary research, encourage innovation, and expand opportunities for engagement in the local research community.

The Science Alliance and its partners, under the umbrella of UT-ORII, will aid UT and ORNL in training and acquiring talented scientists and engineers, as well as providing consistent graduate student support in arenas of global interest.

These initiatives will translate into global scientific and economic impacts, intellectual capacity development, and a prepared future workforce for Tennessee.

Distinguished SCIENTISTS



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, copper- and iron-based high-temperature superconductors, and topological materials including electronic correlations. All these materials and others theoretically studied by his group show promise for both technological applications and for advancing fundamental concepts in condensed matter physics.

In addition to mentoring graduate students, Dagotto's group includes six postdoctoral fellows; Ling-Fang Lin, Yang Zhang, Nitin Kaushal, Pontus Laurell, Arnob Mukherjee, and Bradraj Pandey. Dagotto is the principal investigator (PI) of a multimillion dollar grant from the Department of Energy (DOE) Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. After substantial effort, this DOE grant was successfully renewed for an additional three years, beginning October 1, 2021.

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.

Takeshi Egami, Distinguished Professor in UT's Department of Material 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 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.

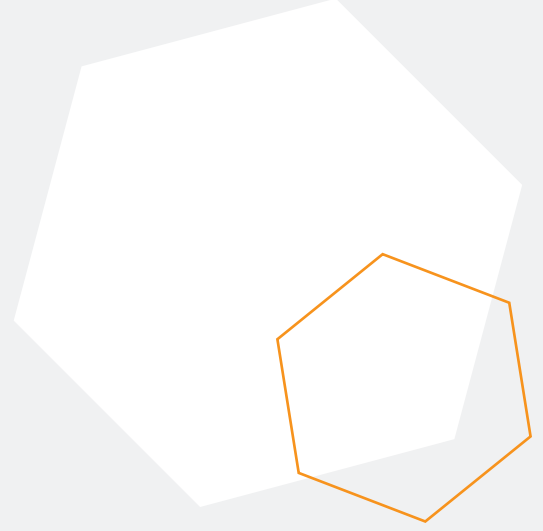
In the last year, Egami's contract from DOE, Basic Energy Sciences was renewed for an additional three years. Egami's team, which includes graduate students Zengquan Wang, Yadukrishna Sarathchandran, Leo Zela, and Rudra Bahadur Bista, demonstrated the feasibility of a new technique to study atomic dynamics in liquid. Additionally, the research group used neutron scattering to solve the long-term mystery of the relaxation mechanism in water that makes microwave ovens work. Egami's research group also includes Jaeyun Moon, postdoctoral fellow, Research Associate Professor Wojciech Dmowski, and Research Assistant Professor Chae Woo Ryu.



Takeshi Egami

External Funding

PRINCIPLE INVESTIGATOR	PROJECT TITLE	FY 22 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	\$90,698
Egami	Fluid Interface Reactions, Structures and Transport (FIRST): Energy Frontier Research Center	\$108,144
Egami	Atomistic Study of Bulk Metallic Glasses	\$101,501



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.

In 2019, 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 are possible, in light of the narrowed topic areas, the LDRD requirement was removed to allow collaborations with any relevant ORNL researcher.

In April 2020 and in response to the global pandemic, the Science Alliance released a call for the JDRD Rapid Response COVID-19 Focus program. The program provided an expanded focus, offering support for projects related to the investigation of COVID-19 in any relevant discipline. Existing JDRD awardees were given the opportunity to apply for second year funding for their existing work based on the original parameters of the 2019 JDRD program.

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.

Dustin Gilbert

MATERIALS SCIENCE & ENGINEERING

Contact with contaminated surfaces is one of the most common ways for illness to spread. A person carrying a pathogen touches something, like a doorknob, then another person touches that object and they can be infected by that pathogen. In between these contacts, the pathogen has to survive on the object, and in a large enough quantity to infect another person. The other common way for pathogens to be transmitted is through the air. Respirators help, but have the same problem, that the captured pathogens survive within the fibers for weeks. Dustin Gilbert, assistant professor of materials science and engineering, wants to make it impossible, or at least unlikely, for pathogens to survive on a surface.

“If you come into contact with a surface containing pathogens, you could get sick from it, so it’s important to have surfaces that are inhospitable environments for pathogens, so they just die quickly rather than being picked up and infecting another person,” said Gilbert.

Most commonly used surfaces are not good at killing pathogens. Pathogens on stainless steel, for example, can take up to five days to die on the surface; on cloth surfaces the timeframe is closer to weeks. However, there are a variety of metals that do a great job killing pathogens. Historically, colloidal silver and brass have both been used for their anti-pathogenic properties. Gilbert’s team wants to leverage the naturally occurring anti-pathogenic properties of these metals to create a more thoroughly inhospitable surface.

“Our idea was to take several of these bioactive metals and put them together into an alloy so effective that whatever pathogen lands on the surface will be attacked by multiple modes of action thanks to the properties of the individual metals,” said Gilbert. “Our goal is to protect against a broader spectrum of pathogens and kill them faster.”

Traditionally, testing these alloys would be a lengthy, laborious process in which each composition is fabricated one piece at a time and tested individually. To overcome this issue Gilbert leveraged his experience in nanotechnology to develop a nanoscale film, enabling him to test thousands of compositions in a single sample.

His team collaborated with Thomas Denes, assistant professor in the Department of Food Science at the



University of Tennessee Institute of Agriculture (UTIA), and Anne Murray, a postdoc in Ecology and Environmental Biology, to conduct pathogen testing on the various alloy compositions. Once complete, the team came together to develop an understanding of the ways in which materials science and biology can work together to address pathogens. A manuscript based on this work has been placed on the Arxiv, document 2205.00886, to facilitate rapid access while the text is under review.

Gilbert also has worked with his ORNL collaborators, Ying Yang and Easo George in the Alloy Behavior and Design Group, to develop a better understanding of high entropy alloys like those used in his project.

Next, his team is working to make this a scalable process using electrochemistry to economically coat large surfaces with highly bioactive alloys. This step also allows the team to prepare nanowires of these bioactive alloys, which can then be used to make metallic filters which have the same antimicrobial properties as the alloys tested before, but now will provide improved protection for respirators. This will also expand the lifetime of respirators, alleviating the crippling shortages experienced during the most recent pandemic. A grant to follow up this research has been submitted to the Army Research Office.

Heidi Goodrich-Blair

MICROBIOLOGY

Since humans began settling into agrarian communities, communicable diseases have been a threat to human health. Part of what makes infectious diseases so dangerous is their ability to evolve and mutate, which can have a variety of effects from easier transmission to more deadly symptoms. The question of how to curtail this evolution has important implications for human health, and is one that Heidi Goodrich-Blair is investigating with her JDRD project. Goodrich-Blair is the David and Sandra White Endowed Professor and Head of the Department of Microbiology.



“Microbial infectious disease is a serious public health issue for the world,” said Goodrich-Blair. “One of the most serious aspects of it is that not only are we getting new emerging infectious diseases, but the ones that we are already familiar with and have been effectively controlling using antibiotics are now becoming resistant to the arsenal of antibiotics we have available to us.”

Outbreaks of infectious diseases have been recorded for thousands of years in communities across the globe, including the black death, the 1918 influenza and more. On average, infectious diseases collectively kill more than 17 million people per year.

Goodrich-Blair is looking for ways to control infectious diseases while sidestepping the rise in antimicrobial resistance. Her JDRD work focuses on using tailocins from bacteriophages. A bacteriophage is a virus that attacks a bacterium by infecting it with the bacteriophage’s DNA. This often results in the destruction of the bacteria, but because of the presence of DNA the process could potentially cause the bacteria to evolve. A tailocin is essentially the part of the bacteriophage used to infect a target bacterium, without the attenuating DNA information.

“Tailocins aren’t going to replicate, they don’t have any nucleic acid material associated with them. They are simply a syringe mechanism. Bacteriophages send these tailocins out and they stick to the outside of a bacterial target cell, then they punch a hole in the cell which then causes it to break down,” said Goodrich-Blair.

While tailocins may be a useful tool for disrupting disease cells without causing them to mutate, the process is not without difficulties. In order for a tailocin to be effective, it must be the right tailocin for the particular bacteria it

is targeting. Goodrich-Blair’s team is investigating the molecules that determine specificity in an attempt to develop a set of molecular tools to help researchers more successfully target bacteria.

“The more you know about that specificity, the more you would be able to tailor and design tailocins that would be able to target a specific range of bacteria,” said Goodrich-Blair.

An important observation that Goodrich-Blair recently discovered is that the tailocin “guidance system” (the part of the structure that defines the specificity for targets) can have extreme variability in the *Xenorhabdus* bacteria and that these organisms are frequently rearranging their genomes to create new types, potentially with new target specificities.

“The organisms are competing with each other --- sort of like an arms race,” Goodrich-Blair explained. This type of tailocin and variable guidance system also exists in strains of pathogenic and probiotic *E. coli*.

Goodrich-Blair said her group plans to exploit the *Xenorhabdus* system to better understand their function in pathogenic *E. coli*, and their potential use to control *E. coli* infections.

Shuai Li

CIVIL & ENVIRONMENTAL ENGINEERING

The role buildings play in spreading disease has been at least suspected since a 1974 study determined a recirculating ventilation system spread measles from one sick student into 14 different classrooms of children. With the arrival of COVID-19 in early 2020, renewed attention has been given to how buildings could accelerate, or potentially inhibit, the spread of illness. Shuai Li, assistant professor in the Department of Civil and Environmental Engineering, is pursuing these questions with his JDRD project.

“There is an urgent need to understand and prevent pathogen transmission within rooms and buildings,” said Li. “In my project, we’re trying to understand what factors are most important both from a building operation and design perspective, and from the human activity perspective.”

Built environments, or buildings, are especially relevant to the spread of disease. The average person spends approximately 90% of their time in built environments, including homes, office buildings, schools, and stores. Not only can these spaces be crowded, but in the case of public buildings, hundreds of people can move through them in the course of a single day, many of whom could be carrying pathogens. In a 2019 study, approximately 90 percent of surveyed adults admitted to knowingly going to work while sick.

According to Li, there are three primary paths of disease transmission: close contact, touching an object someone sick has touched, and airborne contact. While all of these may occur in a built environment, contact with contaminated objects or surfaces and airborne transmission are two areas in which building design and operation interventions could help mitigate the spread of illness.

“We want to know how we can adjust a building’s ventilation or how we can adjust the design and layout of a building to reduce the potential area of contamination,” said Li.

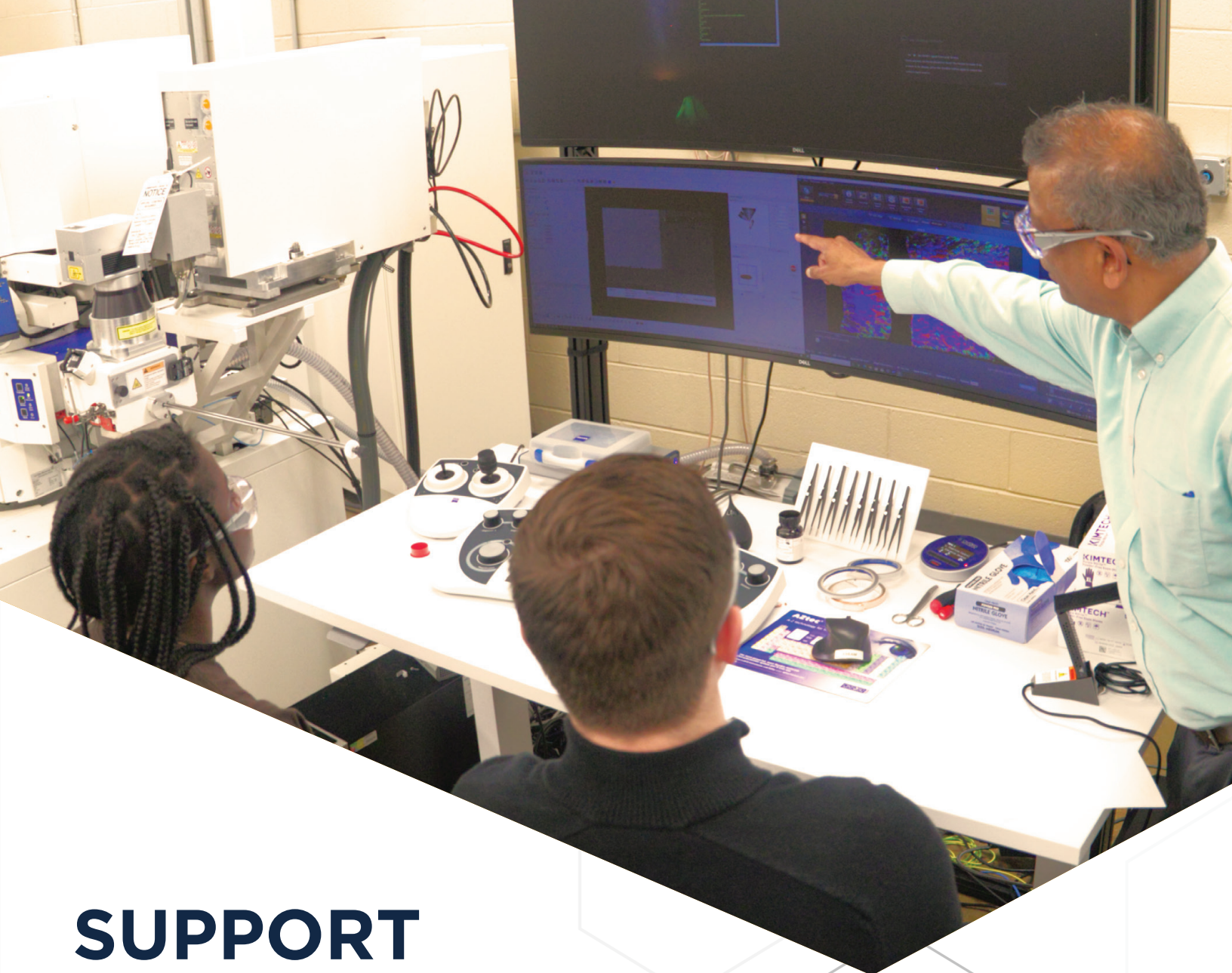
Li’s Co-PI on this project, Civil and Environmental Engineering professor Qiang He, is tasked with collecting and analyzing air and surface samples from a built environment to establish the distribution and characteristics of pathogens in that environment. Li will then use machine learning to establish connections between the attributes of the building and the dynamics of the pathogens found there.



His team is working with both Chris Schadt and Melissa Cregger in the Biosciences Division at ORNL, leveraging their virus modeling capabilities to allow for more accurate assessments of the built environment and the risk of transmission.

Li’s JDRD project grew out of an existing collaboration with He, who Li met when he began his career at UT in 2017. Together they have submitted two proposals to the National Science Foundation and are investigating future joint funding opportunities with Schadt and Cregger.

“Ultimately, we want to develop the knowledge, technology, and tools to combat illness and promote environmental health and hygiene. Environmental health, particularly in the built environment, leads to better human health,” said Li.



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 semi-annual deadlines, in an effort to provide faculty members with greater flexibility and additional access to funding throughout the year. In its second year, the StART program funded eight projects in areas ranging from machine learning in materials science to neuromorphic computing.

John Brantley

CHEMISTRY



Plastic is everywhere – from food and drink containers to kids' toys to car parts.

"We produce billions of tons of plastic waste every year, and many of these materials end up in landfills and they eventually infiltrate the environment," said Brantley, an assistant professor of chemistry.

His StART project focuses on developing new techniques for breaking down plastic waste into useful building blocks that can then be used to make things like fuels, lubricants, or even new plastic materials.

"'Upcycling' is becoming a very active area of research," Brantley said. "We are trying to develop technologies that provide a new pathway for taking an unwanted plastic and converting it into something more valuable."

Brantley says his initial focus – trying to use chemical reactions to change the structures of polymers – shifted based on his team's research over the past year.

"We actually discovered that we could use light and an organic catalyst to transform plastics, or polymers, into smaller units that can be reconfigured into new materials," he said.

Brantley said the chemistry works with both natural sunlight and artificial light.

"And it doesn't require any special precautions to exclude air or water, which makes it a potentially valuable technology for dealing with plastic waste, especially in remote areas.

"In a related development, we found that we could also use electricity (electrochemistry) to achieve very similar outcomes," he said. This facet of their research has been accepted for publication in the Journal of the American Chemical Society.

They are also exploring funding possibilities from the Department of Energy.

Most polymers are petroleum based. Additional oil is required for manufacturing processes and the shipping of finished products.

"If we can figure out a way to extend the life of polymers, we will be getting more bang for our buck from the energy perspective," he said.

Brantley's collaborators include Brian Long, associate professor of chemistry, and Tomonori Saito, a research scientist in ORNL's Chemical Sciences Division, who is interested in energy-related applications of polymers.

Brett Compton

MECHANICAL, AEROSPACE & BIOMEDICAL ENGINEERING



As a high school student, Brett Compton wanted to be a race car driver. He was intrigued by internal combustion engines.

Compton, now an associate professor of mechanical engineering, interned at Porsche while in college and discovered he was more curious about the materials used to make the engines than the engines themselves.

That, combined with a lifelong interest in pottery-making, helped lead him into materials science and mechanical engineering. His StART project involves trying to create ceramic materials with high damage tolerance.

“Ceramic materials maintain good strength and stiffness at elevated temperatures, but they’re lacking in toughness or damage tolerance,” he said.

Think about a coffee mug and a plastic cup: The coffee mug withstands high temperatures while the plastic cup melts. But if they’re dropped, the coffee mug shatters, and the plastic cup bounces.

“It’s a very tricky challenge to balance high strength and high damage tolerance, even more so at high temperature,” Compton said, explaining that he’s using precision additive manufacturing, or 3D printing, to create new damage tolerant hybrid ceramic materials for high temperature applications.

“One of the ways to improve damage tolerance is by adding in weak spots in a controlled pattern,” he said.

A good example is a brick wall. Thanks to the architectural design – individual bricks surrounded by mortar – a crack is confined to zigzagging through the mortar rather than running straight through the bricks and destroying the wall.

Compton and his colleagues are using the brick-and-mortar wall concept. They plan to use additive manufacturing to aluminum oxide beams or “bricks,” then infiltrate them with a “mortar” of phenolic resin that converts to porous carbon when heat treated.

They’ve started by printing and testing tiny aluminum oxide beams with the goal of making the smallest structures possible because they will be the strongest. Next, they’ll add the resin “mortar” and repeat the strength tests.

“If we prove that this works in simple test cases, we can apply the same approach to design a wide range of components with enhanced toughness and excellent temperature stability,” he said.

Compton said potential areas of application include power generation, aerospace, and transportation sectors.

His collaborators include Corson Cramer, a research and development associate at ORNL, and Shradha Agarwal, a research scientist in UT’s Department of Nuclear Engineering, who are considering how the research might be applied to create materials resistant to neutron damage.

Compton’s team is preparing a white paper on their research in hopes of securing outside funding from the Department of Energy.

Kristina Kintziger

PUBLIC HEALTH



As many as 23 million Americans are suffering from “long COVID,” according to the U.S. Government Accountability Office.

“As the COVID-19 pandemic has progressed, we have continued to see people who have been infected with the SARS-CoV-2 virus experiencing long-term symptoms,” said Kristina Kintziger, assistant professor of public health. “By long-term, we mean persistence of symptoms for three months or more from the onset of COVID-19.”

Kintziger’s StART project looks at the effects of long COVID on people in the workplace.

“As COVID-19 is a relatively new illness and has been constantly evolving since its introduction, there is still very little understood about the long-term effects of this disease,” she said. “This quality improvement project will help to shed light on how people experience COVID-19 symptoms in the months and years after their initial infection.”

Kintziger said the symptoms associated with long COVID include brain fog (such as cognitive impairment), headaches, respiratory issues (such as chest pain, shortness of breath, or cough), heart problems (such as palpitations or lightheadedness), stomach issues (such as diarrhea or loss of appetite), skin problems (such as rash or hair loss), and mental health conditions (such as sleep disorders, mood changes, or anxiety), as well as other conditions, including pain, fatigue, or changes in a woman’s menstrual cycle.

“We hope to determine how common these long-term symptoms are in a group of workers and how these symptoms have affected their personal and professional lives,” she said.

The results may help employers understand and improve workplace responses for employees experiencing these long-term COVID symptoms.

Kintziger is collaborating with ORNL’s Health Services Division (HSD) in analyzing quality improvement data.

“(ORNL Staff Psychologist and Reliability Analyst) Mark Waugh and his team in the HSD have conducted an extensive surveillance, testing, and vaccination campaign for the ORNL workforce for most of this pandemic. Data from these activities are to be examined in quality improvement analyses, to include ongoing occupational health surveillance for volunteers experiencing long COVID,” she said.

The team also includes two UT graduate students – Ola Elsakhawy, a doctoral student in comparative and experimental Medicine, and Will Andershock, who is pursuing a Master of Public Health.

Kintziger said the team tries to meet regularly “when the group at HSD are not busy dealing with a new wave of COVID-19 variants.”

The project is still in its initial phase, but “we do hope to publish any important lessons learned from these analyses and possibly turn this into a longer-term project with additional external funds,” Kintziger said.

Eric Lass

MATERIALS SCIENCE & ENGINEERING



Aluminum-cerium (Al-Ce) eutectic alloys are very strong materials that are able to withstand high temperatures tolerated by heavier and more expensive materials, like stainless steel or titanium.

But Al-Ce alloys are so brittle that their commercial uses are limited.

Eric Lass, an assistant professor of materials science and engineering, is leading a StART project to learn how to make these strong, heat-resistant—and cheaper—materials more pliable so they can be more widely used in manufacturing.

Lass said Al-Ce alloys contain a mixture of relatively soft metallic aluminum and a much harder ceramic-like material, called an intermetallic, that contains aluminum and cerium.

“Al-Ce eutectic alloys exhibit very high strengths compared to conventional aluminum alloys,” he said. “Further, they retain their strength up to about 450 degrees Celsius, whereas any other aluminum alloys lose all of its strength above about 200 degrees Celsius.

“But, because they contain a ceramic-like intermetallic, Al-Ce alloys tend to be brittle, and are not ductile,” he said.

“This means that they are difficult to bend or machine into useful geometries for commercial applications.”

Lass and his team hope to engineer more ductile versions of the alloys which can be made into plates, sheets, bars, rods, wires, or other shapes.

“Many components in aerospace and space exploration must be made of steel or titanium due to the temperatures they experience. The successful development of an Al-Ce alloy that could be formed into a sheet for an aircraft skin, structural beam, or similar structure would decrease overall vehicle weight, increase cargo capacity or fuel efficiency, and at the same time reduce cost.”

Lass is working with researchers at ORNL’s Manufacturing Demonstration Facility.

“They are interested in understanding deformation behavior in Al-Ce to help them understand the mechanical properties they see in powder-based additive manufacturing (3-D printing) of Al-Ce alloys, as well as a potential means for producing wire material to use as feedstock for other additive manufacturing technologies,” Lass said.

He will be working with NASA’s Marshall Space Flight Center through the Materials and Manufacturing Joining Innovation Center, an Industry-University Cooperative Research Center supported by the National Science Foundation. Led by Ohio State University with the University of Tennessee, Knoxville as a partner site, the project seeks to develop Al-Ce alloys that can be made in wire form for welding and additive manufacturing applications.

“We also recently submitted a proposal to the DOE Advanced Manufacturing Office with Lawrence Livermore National Laboratory and multiple industrial partners to look at developing wrought Al-Ce alloys (alloys produced through thermo-mechanical processing) for aerospace applications,” he said.

Another proposal for an externally funded research project is forthcoming.

In addition, one of Lass’s graduate students presented a poster at The Materials Society’s 2022 annual meeting, and the team is producing its first paper.

Jian Liu

ELECTRICAL ENGINEERING & COMPUTER SCIENCE



In 2021, more than 1,862 data breaches affected nearly 294 million Americans.

This is troublesome for researchers working with machine learning since they use enormous data sets which may contain sensitive personal information.

Jian Liu, an assistant professor in the Min H. Kao Department of Electrical Engineering and Computer Science, is looking for a reliable way of using federated learning to mitigate the privacy risks to sensitive data in machine learning.

While most machine learning models use centralized training, which requires users to upload their personal data to a remote server, federated learning distributes the training process to a user's device. The model learns from users' data without recording that data onto an external server.

"Recent studies have revealed that private information can still be leaked through shared model updates. In addition, there are billions of mobile devices which can participate in the model learning. We cannot know whether a particular device is trustworthy or if it is malicious," Liu said.

Liu's StART project team is trying to develop attack-resilient and privacy-preserving artificial intelligence models. They have published four papers so far.

"We proposed a method that can serve as a tool for empirically measuring the amount of privacy leakage in federated learning to facilitate the design of more robust defense mechanisms," he said. "We also proposed a secure aggregation rule that can mitigate potential failures and attacks in federated learning. And we designed and evaluated privacy-preserving federated models that can help diagnose Alzheimer's disease and depression based on speech."

Liu's team - which includes Jiaxin Zhang, a staff scientist in ORNL's Computer Science and Mathematics Division, and Luyang Liu, a research scientist at Google - plan to submit a National Science Foundation proposal this year.

PROGRAM FOR ADVANCING COLLABORATIVE TEAMS (PACT) AWARDEE

The Science Alliance was formed to build and enhance relationships between University of Tennessee, Knoxville (UTK) faculty and Oak Ridge National Laboratory (ORNL) scientists and engineers. In keeping with this rich history, the Science Alliance implemented the Program for Advancing Collaborative Teams (PACT) program to provide support for collaborative research endeavors aimed at securing large extramural funding, such as NSF Materials Research Science and Engineering Centers (MRSEC) or NIH RM1 grants.



Nicole McFarlane

ELECTRICAL ENGINEERING & COMPUTER SCIENCE

Imagine if cells and computers could talk.

That might allow doctors to implant patients with a single programmed cell capable of measuring health data, such as blood sugar or hormone levels, and communicating those results in real-time. With no delay for tests or lab work, intervention could be immediate.

Nicole McFarlane, an associate professor of electrical engineering in the Min H. Kao Department of Electrical Engineering and Computer Science, is working on a Program for Advancing Collaborative Teams (PACT) program called “Towards Hybrid Biomicroelectronic Systems” that melds electronics and biology to create biological or environmental sensors that can measure, transmit, and receive information.

“The things that electronics give you is the ability to communicate with the rest of the digital world,” McFarlane said.

Biologist provides the precision: “Biology is way more efficient than anything electronic, so we’re trying to harness the power of biology” by modifying cells so that they can monitor for specific stimuli, communicate information, and receive direction.

“Instead of replicating biology, we want to use it—and talk to it.”

McFarlane is working with other scientists to devise this multi-layered technology.

“I am a circuit designer, not a biologist,” she said.

Her collaborators include Steven Ripp, a research professor in the UT-ORNL Genome Science and Technology program, who is creating cells that communicate via bioluminescence; and Staff Scientist Nickolay Lavrik and Distinguished Research Staff Scientist Scott Retterer, both with ORNL’s Center for Nanophase Materials Science, who are working on nano-size electrodes that will provide the interface between the cells and the electronic circuits that McFarlane is designing.

First, the team is focusing on the science—creating cells that emit light when they encounter a certain stimulus (they’re starting with a thyroid hormone) and outfitting the cells with circuits and electrodes to communicate that information to computers.

After that, the work will expand to other stimuli. And once the science is in place, they’ll focus on wearable and implantable applications.

McFarlane said the team will try to secure external funding from the Department of Defense because military uses are possible and likely to come first. Medical applications, because they require extensive clinical trials and FDA approvals, are likely to take longer.

McFarlane was raised in Trinidad and came to America to attend college. She has a doctorate from the University of Maryland, College Park, and bachelor’s and master’s degrees from Howard University. She has been on the faculty at UT since 2010.



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.” This year, in support of graduate education and research, we funded two colleges within the university. As a result, many students have had occasion to add significantly to the foundation of their future careers through direct support provided by Science Alliance.

Ola Elsakhawy, a doctoral student in comparative and experimental Medicine, and **Will Andershock**, who is pursuing a Master of Public Health have worked with StART faculty Kristina Kitzinger. Their project has focused on long-term symptoms of COVID-19 and how symptoms affect people’s personal and professional lives.

Donnie Hoskins, graduate student in Physics & Astronomy, has collaborated with ORNL scientists on the development of the second Facility for Rare Isotope Beams (FRIB). Hoskins works with instrumentation on the modular array of total absorption spectrometers (MTAS) and is currently working on analysis of the 49K data from the second FRIB Decay station Initiation.

Jian Liu’s StART project is supporting multiple graduate students, working in the field of federated learning. **Yue Cui** is working on privacy preserving depression diagnostics, and students **Zhuohang Li** and **Syed Irfan Ali Meezra** are investigating fairness issues related to federated learning. Both students are engaging in research critical to the development of their careers, as well as the success of the 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 Department of Energy, and NASA. Many of them 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 serve to ensure a foothold for the University of Tennessee, and the state of Tennessee, in the future of the nation’s scientific community.

Student Support by Department

DEPARTMENT	FUNDS	STUDENTS	HIGHLIGHTS
Biology	307,987	58	Students published 18 publications and received awards including the Dr. Cynthia B. Peterson Fellowship, Cokkinias / Fite Award for Outstanding Scholarly Achievement by a Graduate Student 2022, and SEC Emerging Scholars Fellowship 2022.
Chemistry	39,804	9	Nine chemistry students were supported with achievements including publications, NSF affiliation, and oral presentations.
Earth & Planetary Science	39,044	6	Students have a total of 6 publications. Achievements include NSF grants totaling 24,000, two students accepting postdocs, and AGU Student Travel Grant acceptance.
Mathematics	91,769	16	Supported 16 students with more than half maintaining ORNL affiliation and many receiving NSF grants. Awards include R. E. Cline Award, Kuo Fellowship Endowment, GTA Teaching Excellence Fellowship, and Graduate Student Achievement Award.
Physics	194,194	21	Over 75% of students have maintained or are now affiliated with UT and ORNL. Student achievements include five with publications, collaborations with Amazon Web Services, and collaboration of a second FRIB Decay Station Initiator with ORNL researchers
Psychology	9,883	2	Students have published four publications and received honors such as Underrepresented Student/Postdoc Travel Award from the American Society for Pharmacology and Experimental Therapeutics, ASPET Neuropharmacology Division Executive Committee member, and postdoctoral acceptance at Seattle Children's Research Institute.



GRADUATE ADVANCEMENT, TRAINING & EDUCATION

The Science Alliance has a long history of supporting graduate students via assistantships and fellowships awarded by individual departments, now known as the Graduate Advancement, Training, and Education (GATE) program, to support meritorious, collaborative research between the university and ORNL. This program will continue to provide opportunities to students currently studying at our university and will also help recruit the next generation of scientists moving forward. We are now beginning the next phase of this program by offering full graduate research assistantships to students based on the merit of their research. GATE awardees receive a 12-month appointment, including a stipend, tuition waiver, and health insurance.

GATE Awards 2021-2022



MATTHEW BAUCUM

Quantitative Psychology

Matthew Baucum's research focuses on modeling patient response to mechanical ventilation with neuralized HMMs and POMDPs. Mechanical ventilation is a resource-intensive ICU procedure, and 40% of the procedure's duration is spent weaning patients off of the ventilator. Baucum's research aims to reduce unnecessary ventilator use and increase ICU capacity.



KRISTEN BUTLER

Earth & Planetary Sciences

Kristen Butler focuses on soil biogeochemistry, specifically looking at the way manganese cycling impacts the carbon cycle and ultimately global climate change. Butler's research focuses on soils as they are one of the largest terrestrial carbon (C) reservoirs, making the soil carbon pool a key area of study.



ELIZABETH DENISON

Microbiology

Peatlands have been deemed one of the most valuable, as well as one of the most vulnerable, ecosystems on Earth. Elizabeth Dineson is interested in investigating the microscopic organisms that live in association with the dominant plantgenus, Sphagnum (i.e. the Sphagnum microbiome).



ENZO DINGLASAN

Genome Science & Technology

Dinglasan is expanding the sets of tools that can be used to engineer cell-free systems for maximizing protein and metabolite synthesis. The growth of the bioeconomy depends on the integration of biological approaches as green alternatives for commercial production. Bioproduction emerged to address sustainability concerns associated with chemical manufacturing methods that rely on petroleum. The advantage of speed that is offered by cell-free manufacturing will not only hasten our transition into a global bioeconomy, an increasingly urgent need as climate change worsens, it also provides opportunities to sustainably meet surging demands during global emergencies.



DEVON DREY

Nuclear Engineering

Defect formation, defect mobility, and associated disorder profoundly affect the physical properties of many materials and influences material performance in both ambient and extreme environments. Devon Drey's project uses the advanced materials characterization techniques to further our understanding of defect behavior and disordering over a range of length scales in several oxide materials.



RAJESH GHIMIRE

Physics & Astronomy

Rajesh Ghimire focuses on deeper insight into nuclear processes that may answer some of the fundamental questions regarding the creation of all the elements in the universe and the evolution of stars during their lifetime. Ghimire aims to understand the nuclear processes occurring in the cosmos to quantitatively understand the role that different nuclear processes play during the lifetime of a star.



ADRIEN GREEN

Physics & Astronomy

Adrien Green is developing a new optimized error correction protocol for Quantum Key Distribution (QKD) systems. QKD is a communication security protocol that would become necessary for safe internet networking if quantum computers are developed that can break our current public-key encryption system. The optimized system that Green is developing aims to make improvements on the rate of secure-key generation of the system while using low-cost practical hardware.



VISWANATHAN GURUMOORTHY

Genome Sciences & Technology

Viswanathan Gurumoorthy is focused on understanding intrinsically disordered proteins and their structural properties. Intrinsically disordered proteins are present in every form of life performing functions ranging from DNA transcription to cell death. Gurumoorthy hopes their research output would improve our understanding of disordered proteins from a structural perspective and make us realize the underlying principles that could make them functionally diverse.



MOHAMMAD AMINUL HAQUE

Electrical Engineering & Computer Science

Mohammad Aminul Haque completed his PhD under the supervision of our 2021-2022 PACT awardee, Nicole McFarlane. His research interests include semiconductor device fabrication process and analog/mixed-signal integrated circuit design. He worked at ORNL's Center for Nanophase Materials Sciences on developing carbonized electrodes on a complementary metal-oxide-semiconductor (CMOS) platform for biosensing. He also worked on design and characterization of floating gate circuits for noise optimization in photon detection circuits.



MICHELLE LEHMANN

Energy Science & Engineering

Lehmann works on polymer electrolytes and ion exchange membranes for fuel cells and large-scale batteries. Fuel cell technologies are important for clean heavy duty transportation and large-scale batteries are a key technology to enable the widespread adoption of renewable energy resources. Lehmann's research involves designing and synthesizing polymers with improved stability and performance. Lehmann received her PhD from the UT-ORII Bredesen Center's Energy Science and Engineering program in 2022.



SAMARA LEVINE

Nuclear Engineering

Nuclear energy plays a critical role for clean energy production as it accounts for ~10% of the global energy supply and is the second largest source of low-carbon electricity. Samara Levine is developing and qualifying advanced structural materials appropriate for generation IV fission reactor designs that not only must the materials be able to survive a reactor's extreme conditions but also testing of irradiated materials is both costly and time consuming.



ZEYU LIU

Industrial & Systems Engineering

Zeyu Liu's research focuses on mathematical optimization and operations research, especially under parametric uncertainties. His application area includes critical infrastructure, healthcare, transportation, and energy systems. Liu received his doctorate of Philosophy, Industrial Engineering from UT in 2022.



SARAH LOVE

Ecology & Evolutionary Biology

Using the natural laboratory comparison of sky islands and adjacent mountain chains, Sarah Love examines how climate change since the end of the Pleistocene has influenced adaptive demographic processes, plant-soil feedbacks, and plant phenotypes across the entire natural range of the dominant riparian tree, *Populus angustifolia*, narrowleaf cottonwood. Through the GATE Fellowship, Love has partnered with ORNL staff scientist Wellington Muchero to examine the effects of sky island isolation and climatic stressors at the tree genomic level and to identify novel plant-microbial interactions through transcriptomic analysis. Love's research aims to answer questions regarding the climate-induced adaptive capacity of terrestrial organisms driven by community interactions and genetic variation, valuable for understanding the effects of climate change across a large geographic area.



HANG MA

Industrial & Systems Engineering

Hang Ma's research focuses on statistical machine learning, mathematical optimization and scientific computing for modeling, control and optimization of complex dynamic systems ubiquitous in science and engineering. Ma's current work is to develop interpretable machine learning methods to uncover the unknown physical laws in the complex systems, like machining dynamics for smart manufacturing and water electrolysis for green hydrogen production. Ma hopes his work will support the scientific discovery and engineering innovation under the UT-ORNL collaborations and foster industrial participation.



MADDISON MELCHIONNA

Biochemistry, Cellular, & Molecular Biology (BCMB)

Maddison Melchionna's research focuses on understanding the biochemical mechanisms by which bacteria sense changes in their environments and respond to stress. Specifically, she has characterized the function of a widely conserved bacterial membrane protein, which allows cells to balance and maintain homeostasis of membrane energetics, including the transmembrane potential and proton motive force.



FRANCIS OKEJIRI

Chemistry

Francis Okejiri's research focuses on sonochemically synthesizing different classes of advanced material including high-entropy alloys, high-entropy metal oxides, supported single-atom alloy catalysts, etc. for catalysis applications. Traditional solid-state reaction and solution-mediated processes commonly used for the synthesis of these materials, at some stage, require calcination in extreme temperature conditions. Okejiri's sonochemical-based method is not limited by this temperature requirement and can synthesize high-entropy nanocrystals – a process that will otherwise require high-temperature calcination for an extended period.



NICK OLDHAM

Entomology & Plant Pathology

Nick Oldham is a pollinator ecologist that focuses on the relationship between wetlands and pollinators. In particular, Oldham has examined how land use and anthropogenic disturbance affect wetlands and their local plant and pollinator communities. Hoverflies are of special interest, which are extremely important pollinators but don't get as much attention as bees. Current research from Oldham shows that these relationships are quite complex and dependent on the level of disturbance. Oldham is currently a pollinator support subcontractor for the Natural Resources Management Program at ORNL, aiming to improve pollinator habitat and promote biodiversity.



SREYA PALADUGU

Materials Science & Engineering

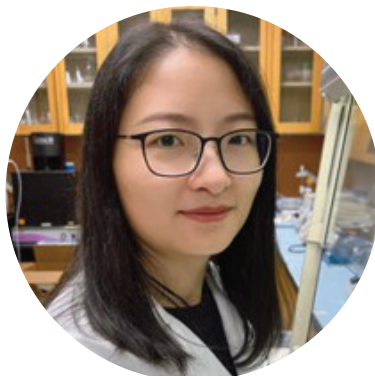
Sreya is investigating the structure of metal oxide nano catalysts in-situ, with the objective of understanding how these materials evolve under conditions that mimic real automotive catalytic converters. She hopes her work will contribute to the discovery of industrially relevant materials for energy applications.



TYLER STEINER

Nuclear Engineering

A lifetime of natural curiosity brought Tyler to the field of nuclear engineering for space applications. Nuclear thermal propulsion has been chosen by NASA to send humans to Mars, but a testbed for simulating the specific conditions this mission will experience does not yet exist. Tyler's research will contribute to the development of such a testbed in an ongoing UT-ORNL collaboration.



HUIHUI SUN

Biosystems Engineering & Soil Science

Huihui Sun focuses on pore hydrology control on the retention and dispersion of bacteria and viruses in soil. Sun's research investigates the impact of soil porous networks on physical interactions of viruses and their hosts in soil ecosystems using small angle X-ray and neutron scattering techniques. The results will provide insight into the role of bacteria and viruses in biologically-mediated processes affecting health and enhancing soil productivity.



XIN WEN

Physics & Astronomy

Through collaboration with ORNL and National High Magnetic Field Laboratory, Wen's developing a new technique to visualize flow in extreme conditions using neutrons and liquid helium. His work seeks to effectively quantify and test theoretical models that describe the development, intensity and internal structure of turbulent flow. His work also broadens the application of neutron beams.



YI YANG

Materials Science & Engineering

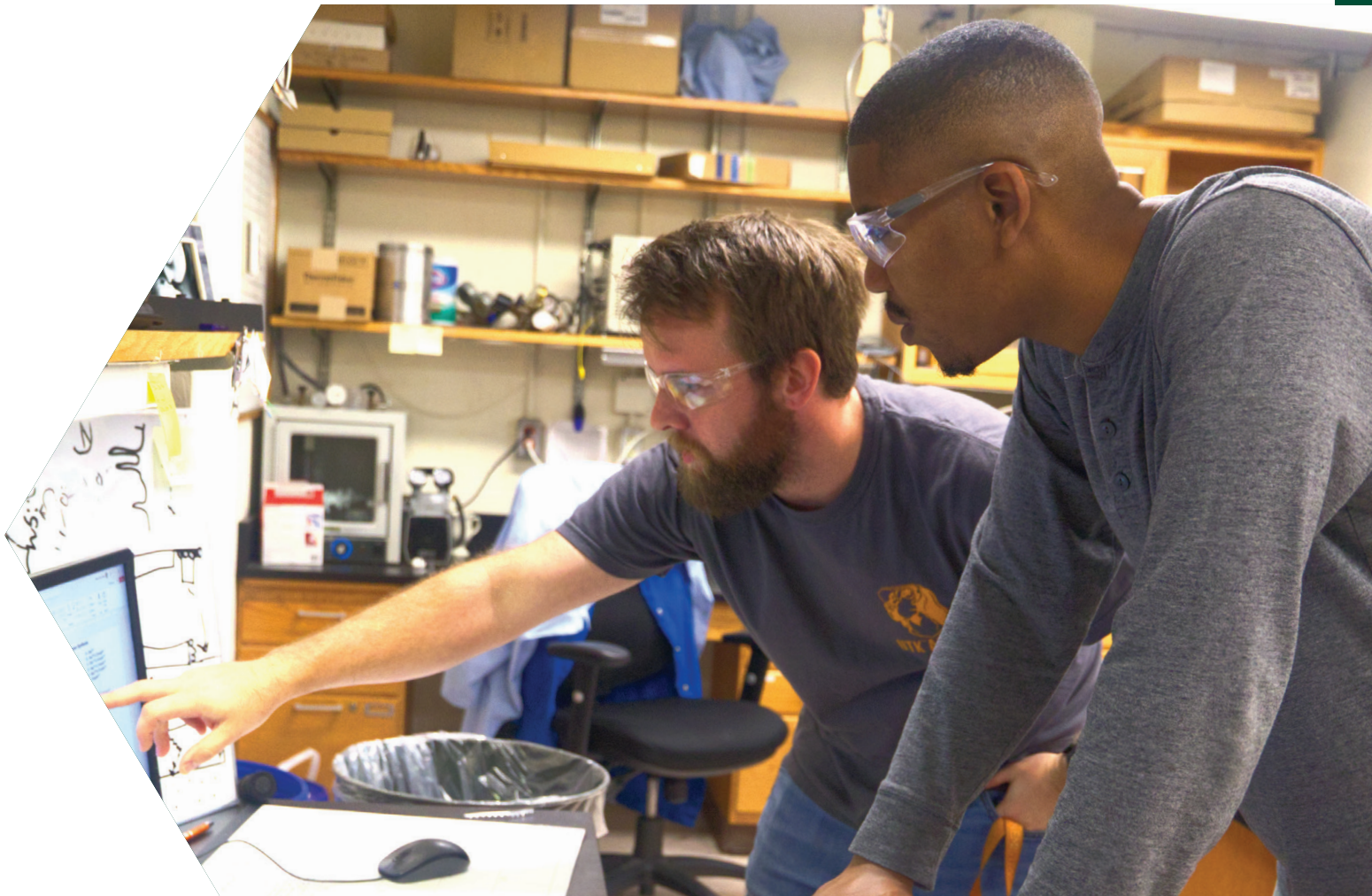
Yi Yang researches residual stress and lifetime prediction in weldments for pipeline systems. Yang uses a simulation model to predict microstructure evolution and failure location, which is impossible for experiments to mimic due to time limitations. This project can provide guidance for industry that heavily uses pipeline systems.



HAO ZHANG

Physics & Astronomy

Hao Zhang researches theoretical condensed matter physics with an emphasis on quantum magnetism. In particular, Zhang's interest is in the novel states of matter and the dynamical response in frustrated quantum materials. Zhang has developed some generalized notations in the field of quantum magnetism in their Ph.D. dissertation. These generalized notations provide powerful theoretical tools for modeling diffuse and inelastic neutron scattering experiments performed at the Neutron Scattering Division of ORNL.





STUDENT MENTORING AND RESEARCH TRAINING

In an effort to deepen its existing commitment to student support, the Science Alliance launched the Student Mentoring and Research Training (SMaRT) program for undergraduates in 2020. SMaRT interns have the unique opportunity to work with researchers from UT and Oak Ridge National Laboratory for 10 weeks over the summer, gaining firsthand research experience in emerging fields, such as advanced manufacturing, energy storage, transportation, quantum information sciences and data sciences.

The ultimate goal with the SMaRT program: to recruit our top interns to UT for grad school and to build their careers in Tennessee.

In 2020, the first year of program, most of our interactions were virtual to comply with UT and ORNL COVID-19 safety precautions. Our 2021 cohort of 18 interns, still bound by a number of safety precautions, was able to more fully engage in the research process with faculty mentors at UT, but not at ORNL. In May 2022, with most of the COVID restrictions lifted, we more than doubled our number

of interns to 41, recruiting some of the nation's best and brightest undergraduates across the country and Canada.

Throughout the summer, UT and ORNL researchers, including several of our UT-ORNL Governor's Chairs, serve as mentors to our interns. Graduate students work daily with the interns, sharing their own graduate school experiences and helping the undergraduates better understand and evaluate their graduate school options at UT and future career opportunities.

Our interdisciplinary atmosphere gives interns a "team science" experience, an increasingly important platform for research. At the conclusion of their research experience, interns work with their faculty and graduate student mentors to develop posters and formal presentations describing the research they conducted over the course of the program. The interns individually deliver their presentation before a room filled with their peers, researchers and others from UT and ORNL, and family members, at our annual two-day SMaRT Symposium.

SMaRT Student Support

The Science Alliance's support of students engaging in research extends beyond graduate students. With the 2020 launch of the SMaRT program, Science Alliance funds are also bolstering research opportunities for undergraduate students.

Through this 10-week summer program, SMaRT interns are mentored and trained by some of the nation's top scientists, many of whom serve joint research appointments at UT and ORNL. They are engaged in some of the most cutting-edge research in the world.

UTK-ORNL governor's chair Suresh Babu's group; **Anthony Diaz-Huemme, Connor Vernachio, D'Mia Dent** and **Sumandeep Kaur** worked at ORNL's Manufacturing Demonstration Facility. Diaz-Huemme, Vernachio, Dent, and Kaur worked on better understanding additive manufacturing pertaining to keyhole stability and tensile property variation.

Mechanical, Aerospace, and Biomedical Engineering Professor Tony Schmitz's interns: **Ian Kinsel, Kamren Sargent**, and **Kyle Sprecker**, conducted their research in the Machine Tool Research Center at the University of Tennessee, Knoxville. Kinsel, Sargent, and Sprecker worked on creating a MELD L3 Loading Automation to semi-automate reloading metal feedstock to limit human intervention and increase efficiency in the reloading process.

Alana Wells, Daniel Hicks, and T'Lexus Gantt spent their internship researching Alzheimer's through RNA sequencing and ion mobility mass spectrometry with Dr. Thanh Do, assistant professor of chemistry.

Lillie Hunter and **Isaac Krosschell** worked with Mina Sartipi, a researcher at the University of Tennessee at Chattanooga on groundbreaking research focusing on transit efficiency and making traffic safer. Hunter and Krosschell researched a road use detection and tracking system along the MLK Smart Corridor in Chattanooga, TN.

SMaRT interns investigate areas critical to the future of both the university and the state of Tennessee, and gain skills and knowledge integral to a career in research. They also receive professional development instruction in a variety of areas and are provided a solid foundation to continue building their research goals.



Undergraduate Support

DEPARTMENT	FUNDS	STUDENTS
Biosystems Engineering and Soil Science	\$1,535.00	1
Center for Information Technology Research	\$204.00	1
Clinical Pharmacy	\$1,867.50	1
Civil and Environmental Engineering	\$592.00	2
Diversity and Engagement	\$320.00	1
Electrical Engineering and Computer Science	\$25,964.10	6
Industrial and Systems Engineering	\$101.25	1
Materials Science and Engineering	\$130.20	1
Mechanical, Aerospace, & Biomedical Engineering	\$4,937.50	8

Distinguished Scientists

Elbio Dagotto

Okamoto, S., Mohanta, N., **Dagotto, E.**, & Sheng, D. N. (2022). Topological flat bands in a kagome lattice multiorbital system, *Communications Physics* 5, 198

Laurell, P., Scheie, A., Alan Tennant, D., Okamoto, S., Alvarez, G., & **Dagotto, E.** (2022). Magnetic excitations, nonclassicality, and quantum wake spin dynamics in the Hubbard chain, *Phys. Rev. B* 106, 085110

Mohanta, N. & **Dagotto, E.** (2022). Interfacial phase frustration-stabilized unconventional skyrmion crystals, *npj Quantum Materials* 7, 76

Soni, R., Kaushal, N., Sen, C., Reboredo, F. A., Moreo, A., & **Dagotto, E.** (2022). Estimation of biquadratic and bicubic Heisenberg effective couplings from multiorbital Hubbard models, *New J. Phys.* 24, 073014

Lin, L.-F., Soni, R., Zhang, Y., Gao, S., Moreo, A., Alvarez, G., Christianson, A. D., Stone, M. B., & **Dagotto, E.** (2022). Electronic structure, magnetic properties, and pairing tendencies of the copper-based honeycomb lattice $\text{Na}_2\text{Cu}_2\text{TeO}_6$, *Phys. Rev. B* 105, 245113

Do, S.-H., Kaneko, K., Kajimoto, R., Kamazawa, K., Stone, M. B., Lin, J. Y. Y., Itoh, S., Masuda, T., Samolyuk, G. D., **Dagotto, E.**, Meier, W. R., Sales, B. C., Miao, H., & Christianson, A. D. (2022). Damped Dirac magnon in the metallic kagome antiferromagnet FeSn , *Phys. Rev. B* 105, L180403

Zhang, Y., Lin, L. -F., Moreo, A., Maier, T. A., Alvarez, G., & **Dagotto, E.** (2022). Strongly anisotropic electronic and magnetic structures in oxide dichlorides RuOCl_2 and OsOCl_2 , *Phys. Rev. B* 105, 174410

Maier, T.A. & **Dagotto, E.** (2022). Coupled Hubbard ladders at weak coupling: Pairing and spin excitations, *Phys. Rev. B* 105, 054512

Mazza, A., Skoropata, E., Sharma, Y., Lapano, J., Heitmann, T. W., Musico, B. L., Keppens, V., Gai, Z., Freeland, J. W., Charlton, T. R., Brahlek, M., Moreo, A., **Dagotto, E.**, & Ward, T. Z. (2022). Designing Magnetism in High Entropy Oxides, *Adv. Sci.* 2200391.

Lin, L.-F., Zhang, Y., Alvarez, G., Herbrych, J., Moreo, A., & **Dagotto, E.** (2022). Prediction of orbital selective Mott phases and block magnetic state in the quasi-one-dimensional iron chain $\text{CeO}_2\text{FeSe}_2$ under hole and electron doping, *Phys. Rev. B* 105, 075119

Zhang, Y., Lin, L. -F., Moreo, A., & **Dagotto, E.** (2022). Theoretical study of the crystal and electronic properties of $\alpha\text{-RuI}_3$, *Phys. Rev. B* 105, 085107

Zhang, Y., Lin, L. -F., Moreo, A., & **Dagotto, E.** (2022). Electronic and magnetic properties of quasi-one-dimensional osmium halide OsCl_4 , *Appl. Phys. Lett.* 120, 023101

Kaushal, N., Herbrych, J., Alvarez, G., & **Dagotto, E.** (2021). Magnetization dynamics fingerprints of an excitonic condensate $(t_2g)^4$ magnet, *Phys. Rev. B* 104, 235135

Pandey, B., Alvarez, G., & **Dagotto, E.** (2021). Excitonic wave-packet evolution in a two-orbital Hubbard model chain: A real-time real-space study, *Phys. Rev. B* 104, L220302

Mohanta, N., Ok, J. M., Zhang, J., Miao, H., **Dagotto, E.**, Lee, H.N., & Okamoto, S. (2021). Semi-Dirac and Weyl fermions in transition metal oxides, *Phys. Rev. B* 104, 235121

Soni, R., Sanyal, A. B., Kaushal, N., Okamoto, S., Moreo, A., & **Dagotto, E.** (2021). Multitude of topological phase transitions in bipartite dice and Lieb lattices with interacting electrons and Rashba coupling, *Phys. Rev. B* 104, 235115

Zhang, Y., Hu, W. -J., **Dagotto, E.**, & Gong, S. (2021). Fragility of the nematic spin liquid induced by diagonal couplings in the square-lattice $\text{SU}(3)$ model, *Phys. Rev. B* 104, 195135

Mazza, A., Skoropata, E., Lapano, J., Zhang, J., Sharma, Y., Musico, B. L., Keppens, V., Gai, Z., Brahlek, M. J., Moreo, A., Gilbert, D. A., **Dagotto, E.**, & Ward, T. Z. (2021). Charge doping effects on magnetic properties of single-crystal $\text{La}_{1-x}\text{Sr}_x(\text{Cr}_{0.2}\text{Mn}_{0.2}\text{Fe}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2})\text{O}_3$ ($0 \leq x \leq 0.5$) high-entropy perovskite oxides, *Phys. Rev. B* 104, 094204

Zhang, Y., Lin, L. -F., Alvarez, G., Moreo, A., & **Dagotto, E.** (2021). Magnetic states of quasi-one-dimensional iron chalcogenide Ba_2FeS_3 , *Phys. Rev. B* 104, 125122

Lin, L.-F., Zhang, Y., Alvarez, G., Moreo, A., & **Dagotto, E.** (2021). Origin of insulating ferromagnetism in iron oxychalcogenide $\text{CeO}_2\text{FeSe}_2$, *Phys. Rev. Letters* 127, 077204

Zhang, Y., Lin, L. -F., Moreo, A., & **Dagotto, E.** (2021). Orbital-selective Peierls phase in the metallic dimerized chain MoOCl_2 , *Phys. Rev. B* 104, L060102

Myoung-Woo, Y., Tornos, J., Sander, A., Lin, L. -F., Mohanta, N., Peralta, A., Sanchez-Manzano, D., Gallego, F., Haskel, D., Freeland, J. W., Keavney, D. J., Choi, Y., Stremper, J., Wang, X., Cabero, M., Vasili, H. B., Valvidares, M., Sanchez-Santolino, G., Gonzalez-Calbet, J. M., Rivera, A., Leon, C., Rosenkranz, S., Bibes, M., Barthelemy, A., Anane, A., **Dagotto, E.**, Okamoto, S., te Velthuis, S. G. E., Santamaria, J., & Villegas, J. E. (2021). Large intrinsic anomalous Hall effect in SrIrO_3 induced by magnetic proximity effect, *Nature Communications* 12, 3283

Mohanta, N., Okamoto, S., & **Dagotto, E.** (2021). Skyrmion Control of Majorana States in Planar Josephson Junctions, *Comm. Phys.* (Nature) 4, 163

Sroda, M., **Dagotto, E.**, & Herbrych, J. (2021). Quantum magnetism of iron-based ladders: blocks, spirals, and spin flux, *Phys. Rev. B* 104, 045128

Pandey, B., Soni, R., Lin, L. -F., Alvarez, G., & **Dagotto, E.** (2021). Intertwined charge, spin, and pairing orders in doped iron ladders, *Phys. Rev. B* 103, 214513

Herbrych, J., Sroda, M., Alvarez, G., Mierzejewski, M., & **Dagotto, E.** (2021). Interaction-induced topological phase transition and Majorana edge states in low-dimensional orbital-selective Mott insulators, *Nature Communications* 12, 2955

Lin, L.-F., Kaushal, N., Sen, C., Christianson, A. D., Moreo, A., & **Dagotto, E.** (2021). Oxygen magnetic polarization, nodes in spin density, and zigzag spin order in oxides, *Phys. Rev. B* 103, 184414

Zhang, Y., Lin, L. -F., Moreo, A., Alvarez, G., & **Dagotto, E.** (2021). Peierls transition, ferroelectricity, and spin-singlet formation in the monolayer VOI_2 , *Phys. Rev. B* 103, L121114

Lin, L.-F., Kaushal, N., Zhang, Y., Moreo, A., & **Dagotto, E.** (2021). Orbital ordering in the layered perovskite material CsVF_4 , *Phys. Rev. Materials* 5, 025001

Zhang, Y., Kaushal, N., Soni, R., Lin, L. -F., Hu, W. -J., Alvarez, G., & **Dagotto, E.** (2021). Origin of the Magnetic and Orbital ordering in $\alpha\text{-Sr}_2\text{CrO}_4$, B. Pandey, *Phys. Rev. B* 103, 045115

Distinguished Scientists, Continued

Takeshi Egami

Egami, T. & Ryu, C. W. (2022). Structural Principles in Liquids and Glasses: Bottom-Up or Top-Down. *Frontiers in Materials*, 9. <https://doi.org/10.3389/fmats.2022.874191>

Lieou, C. & **Egami, T.** (2022). Mean-field model for the Curie-Weiss temperature dependence of coherence length in metallic liquids. *Physical Review E*, 105(4-1), 044135–044135. <https://doi.org/10.1103/PhysRevE.105.044135>

Novak, E., Daemen, L., Ramirez-Cuesta, A. J., Cheng, Y., Smith, R., **Egami, T.**, & Jalarvo, N. (2022). Uncovering the hydride ion diffusion pathway in barium hydride via neutron spectroscopy. *Scientific Reports*, 12(1), 6194–6194. <https://doi.org/10.1038/s41598-022-10199-8>

Zella, L., Moon, J., Keffer, D., & **Egami, T.** (2022). Transient nature of fast relaxation in metallic glass. *Acta Materialia*, 239. <https://doi.org/10.1016/j.actamat.2022.118254>

Wang, H., Dmowski, W., Tong, Y., Wang, Z., Yokoyama, Y., Ketkaew, J., Schroers, J., & **Egami, T.** (2022). Nonaffine Strains Control Ductility of Metallic Glasses. *Physical Review Letters*, 128(15), 155501–155501. <https://doi.org/10.1103/PhysRevLett.128.155501>

Shinohara, Y., Ivanov, A. S., Maltsev, D., Granroth, G. E., Abernathy, D. L., Dai, S., & **Egami, T.** (2022). Real-Space Local Dynamics of Molten Inorganic Salts Using Van Hove Correlation Function. *The Journal of Physical Chemistry Letters*, 13(25), 5956–5962. <https://doi.org/10.1021/acs.jpclett.2c01230>

Zarkadoulas, E., Shinohara, Y., & **Egami, T.** (2022). X-ray free-electron laser heating of water at picosecond time scale. *Physical Review Research*, 4(1). <https://doi.org/10.1103/PhysRevResearch.4.013022>

Lokshin, K., Mitchell, D., Lobanov, M. V., Struzhkin, V., & **Egami, T.** (2022). Synthesis and Characterization of Pure Infinite Layer Ni⁺ Nickelates: LnNiO₂ (Ln = La, Nd, Pr) and La₃Ni₂O₆. *ECS Journal of Solid State Science and Technology*, 11(4). <https://doi.org/10.1149/2162-8777/ac6623>

Lokshin, K., Mitchell, D., Lobanov, M. V., Struzhkin, V., & **Egami, T.** (2022). Synthesis and Characterization of Pure Infinite Layer Ni + Nickelates: LnNiO₂ (Ln = La, Nd, Pr) and La₃Ni₂O₆. *ECS Journal of Solid State Science and Technology*, 11(4), 44008–. <https://doi.org/10.1149/2162-8777/ac6623>

Matsumoto, R., Thompson, M. W., Vuong, V. Q., Zhang, W., Shinohara, Y., van Duin, A. C. T., Kent, P. R. C., Irle, S., **Egami, T.**, & Cummings, P. T. (2021). Investigating the Accuracy of Water Models through the Van Hove Correlation Function. *Journal of Chemical Theory and Computation*, 17(10), 5992–6005. <https://doi.org/10.1021/acs.jctc.1c00637>

Moon, J. & **Egami, T.** (2021). Enhancing elastic properties of single element amorphous solids through long-range interactions. *Applied Physics Letters*, 119(5), 51901–. <https://doi.org/10.1063/5.0056108>

Oh, H., Obadrakh, K., Ikeda, Y., Mu, S., Körmann, F., Sun, C. -J., Ahn, H. S., Yoon, K. N., Ma, D., Tasan, C. C., **Egami, T.**, & Park, E. S. (2021). Element-resolved local lattice distortion in complex concentrated alloys: An observable signature of electronic effects. *Acta Materialia*, 216(C), 117135–. <https://doi.org/10.1016/j.actamat.2021.117135>

Ryu, C.W. & **Egami, T.** (2021). Medium-range atomic correlation in simple liquids. I. Distinction from short-range order. *Physical Review E*, 104(6), 064109–064109. <https://doi.org/10.1103/PhysRevE.104.064109>

Egami, T. & Ryu, C. W. (2021). Medium-range atomic correlation in simple liquids. II. Theory of temperature dependence. *Physical Review E*, 104(6), 064110–064110. <https://doi.org/10.1103/PhysRevE.104.064110>

Egami, T. (2021). What does the structure of liquid mean? *Acta Crystallographica. Section A, Foundations and Advances*, 77(a2), C458–C458. <https://doi.org/10.1107/S010876732109228X>

Matsumoto, R., Thompson, M. W., Vuong, V. Q., Zhang, W., Shinohara, Y., van Duin, A. T., Kent, P. C., Irle, S., **Egami, T.**, & Cummings, P. T. (2021). Investigating the Accuracy of Water Models through the Van Hove Correlation Function. *Journal of Chemical Theory and Computation*, 17(10).

Jeong, S.G., Kim, J., Seo, A., Park, S., Jeong, H. Y., Kim, Y. -M., Lauter, V., **Egami, T.**, Han, J. H., & Choi, W. S. (2022). Unconventional interlayer exchange coupling via chiral phonons in synthetic magnetic oxide heterostructures. *Science Advances*, 8(4), eabm4005–eabm4005. <https://doi.org/10.1126/sciadv.abm4005>

Novak, E., Daemen, L., Page, K., Neufeind, J., Everett, M., **Egami, T.**, & Jalarvo, N. (2021). Temperature Dependent Local Atomic Structure and Vibrational Dynamics of Barium Hydride and Calcium Hydride. *Journal of Physical Chemistry C*, 125(44), 24328–24339. <https://doi.org/10.1021/acs.jpcc.1c08070>



GATE Publications

Hang Ma

Ma, H., Zhang, C., & Shi, Z. (2022). "A Simulation Optimization-Aided Learning Method for Design Automation of Scheduling Rules", IEEE International Conference on Automation Science and Engineering (CASE)

Mohammad Aminul Haque

Haque, M.A., Lavrik, N. V., Hensley, D., Briggs D. P., & McFarlane, N. (2021). "Carbonized Polymer for Joule Heating Processing Towards Biosensor Development," 2021 43rd Annual International Conference of the IEEE Engineering in Medicine & Biology Society (EMBC) doi: 10.1109/EMBC46164.2021.9630908.

Hesari, S., Haque, M.A., & McFarlane, N. (2021). A comprehensive survey of readout strategies for sipms used in nuclear imaging systems. Photonics, 8(7), 266-. <https://doi.org/10.3390/photonics8070266>

Nitesh Shah

Shah, N.R. & Cherry, C. R. (2022). The Chance of Getting Struck by a Car on an E-Scooter Is Twice as High at Night. Findings, June. <https://doi.org/10.32866/001c.36195>.

Ziedan, A., Shah, N.R., Brakewood, C., & Cherry, C. R. (2022). A Method for Placing Shared E-Scooters Corrals Near Transit Stops. Proceedings of the 101st Annual Meeting of the Transportation Research Board, Washington, DC.

Ziedan, A., Shah, N.R., Wen, Y., Brakewood, C., Cherry, C. R., & Cole, J. (2021). Complement or compete? The effects of shared electric scooters on bus ridership. Transportation Research Part D: Transport and Environment, 101, 103098

Shah, N.R., & Cherry, C. R. (2021). Different Safety Awareness and Route Choice between Frequent and Infrequent Bicyclists: Findings from Revealed Preference Study Using Bikeshare Data. Transportation Research Record. <https://doi.org/10.1177/03611981211017136>

Shah, N.R., Aryal, S., Wen, Y., & Cherry C. R. (2021). Comparison of motor vehicle-involved e-scooter and bicycle crashes using standardized crash typology. Journal of Safety Research 77: 217-228

Zeyu Liu

Liu, Z., Li, X., & Khojandi, A. (2022). The flying sidekick traveling salesman problem with stochastic travel time: A reinforcement learning approach. Transportation Research Part E: Logistics and Transportation Review, 164, 102816.

Liu, Z., Khojandi, A., Li, X., Mohammed, A., Davis, R. L., & Kamaleswaran, R. (2022). A Machine Learning-Enabled Partially Observable Markov Decision Process Framework for Early Sepsis Prediction. INFORMS Journal on Computing. To appear.

Lyu, Z., **Liu, Z.**, Khojandi, A., & Yu, A. J. (2022). Q-learning and traditional methods on solving the pocket Rubik's cube. Computers & Industrial Engineering, 171, 108452.

Kizito, R., **Liu, Z.**, Li, X., & Sun, K. (2022). Multi-stage stochastic optimization of islanded utility-microgrids design after natural disasters. Operations Research Perspectives, 9, 100235.

Kizito, R., **Liu, Z.**, Li, X., & Sun, K. (2021). Stochastic optimization of distributed generator location and sizing in an islanded utility microgrid during a large-scale grid disturbance. Sustainable Energy, Grids and Networks, 27, 100516.

Liu, Z., Khojandi, A., Mohammed, A., Li, X., Chinthala, L. K., Davis, R. L., & Kamaleswaran, R. (2021). HeMA: A hierarchically enriched machine learning approach for managing false alarms in real time: A sepsis prediction case study. Computers in biology and medicine, 131, 104255.

Liu, C., Chen, H., Li, X., & **Liu, Z.** (2021). A scheduling decision support model for minimizing the number of drones with dynamic package arrivals and personalized deadlines. Expert Systems with Applications, 167, 114157.

Huhui Sun

Sun, H., Sun, Y., Jin, M., Ripp, S. A., Sayler, G. S., & Zhuang, J. (2022). Domestic plant food loss and waste in the United States: Environmental footprints and mitigation strategies. Waste Management, 150, 202-207

Zhuang, J., **Sun, H.**, Sayler, G., Kline, K., Dale, V., Jin, M., Yu, G., Fu, B., & Löffler, F. (2021). Food-Energy-Water Crises in the United States and China: Commonalities and Asynchronous Experiences Support Integration of Global Efforts. Environmental Science & Technology, 55(3), 1446-1455

Sun, Y., Im, J., Shobnam, N., Fanourakis, S., He, L., Erickson, P., **Sun, H.**, Zhuang, J., & Löffler, F. (2021). Degradation of adsorbed bisphenol A (BPA) by soluble Mn(III). Environmental Science & Technology, 55(19), 13014-13023

Michelle Lehmann

Lehmann M., Yang, G., Nanda, J., & Saito, T. (2022). Unraveling Ion Transport in Trifluoromethanesulfonimide Pentablock Copolymer Membranes in Nonaqueous Electrolytes. Macromolecules, 55(17), 7740-7751. <https://doi.org/10.1021/acs.macromol.2c00513>

Lehmann, M., Yang, G., Self, E. C., Li, B., Delnick, F. M., Nanda, J., & Saito, T. (2019). Mechanically Robust Crosslinked Membranes for Non-Aqueous Redox Flow Batteries. Meeting Abstracts (Electrochemical Society), MA2019-01(3), 450-450. <https://doi.org/10.1149/MA2019-01/3/450>

Zhang, Y., Yang, G., **Lehmann, M.**, Wu, C., Zhao, L., Saito, T., Liang, Y., Nanda, J., & Yao, Y. (2021). Separator Effect on Zinc Electrodeposition Behavior and Its Implication for Zinc Battery Lifetime. Nano Letters, 21(24), 10446-10452. <https://doi.org/10.1021/acs.nanolett.1c03792>

Chen, X., Zhang, Y., Merrill, L. C., Soulen, C., **Lehmann, M.**, Schaefer, J. L., Du, Z., Saito, T., & Dudney, N. J. (2021). Gel composite electrolyte - an effective way to utilize ceramic fillers in lithium batteries. Journal of Materials Chemistry. A, Materials for Energy and Sustainability, 9(1), 6555-6566. <https://doi.org/10.1039/d1ta00180a>

Enzo Dinglasan

Dinglasan, J.L.N., Reeves, D. T., Hettich, R. L., & Doktycz, M. J. (2021). Liquid Chromatography Coupled to Refractive Index or Mass Spectrometric Detection for Metabolite Profiling in Lysate-based Cell-free Systems. Journal of Visualized Experiments (175), e62852, doi:10.3791/62852

Garcia, D., **Dinglasan, J.L.N.**, Shrestha, H.K., Abraham, P.E. Hettich, R.L., & Doktycz, M.J. (2021). A lysate proteome engineering strategy for enhancing cell-free metabolite production. Metabolic Engineering Communications. 12 e00162, doi: 10.1016/j.mec.2021.e00162

Maddison Melchionna

Melchionna, M., Gullett, J. M., Bouveret, E., Shrestha, H. K., Abraham, P. E., Hettich, R. L., & Alexandre, G. (2022). Bacterial Homologs of Progesterone and AdipoQ Receptors (PAQRs) Affect Membrane Energetics Homeostasis but Not Fluidity. *J Bacteriol.* 204 (4): e0058321. doi: 10.1128/jb.00583-21.

Hao Zhang

Dahlbom, D., Miles, C., **Zhang, H.**, Batista, C. D., & Barros, K. (2022). Langevin dynamics of generalized spins as $SU(N)$ coherent states. *arXiv*, 2209.01265

Scheie, A.O., Kamiya, Y., **Zhang, H.**, & Lee, S. (2022). Non-linear magnons in the $1/3$ magnetization plateau of a proximate quantum spin liquid. *arXiv*, 2207.14785

Do, S.-H., **Zhang, H.**, Dahlbom, D., Williams, T.J., Garlea, O., Hong, T., Cheong, S.-W., Park, J.-H., Barros, K., Batista C., & Christianson, A. (2022). Understanding temperature-dependent $SU(3)$ spin dynamics in the antiferromagnet $Ba_2FeSi_2O_7$. *arXiv*, 2205.11770

Zhang, H., Wang, Z., Dahlbom, D., Barros, K., & Batista C.D. (2022). CP2 Skyrmions and Skyrmion Crystals in Realistic Quantum Magnets. *arXiv*, 2203.15248

Dahlbom, D., **Zhang, H.**, Miles, C., Bai, X., Batista, C.D., & Barros, K. (2022). Geometric integration of classical spin dynamics via a mean-field Schrödinger equation. *Phys. Rev. B*, 106, 054423

Bai, X., Zhang, S.-S., **Zhang, H.**, Dun, Z., Phelan, W. A., Garlea, V. O., Mourigal, M., & Batista, C. D. (2021). Instabilities of heavy magnons in an anisotropic magnet. *arXiv*, 2107.05694

Zhang, H., & Batista, C.D. (2021). Classical spin dynamics based on $SU(N)$ coherent states. *Phys. Rev. B*, 104, 104409

Do, S.-H., **Zhang, H.**, Williams, T. J., Hong, T., Garlea, V. O., Rodriguez-Rivera, J. A., Jang, T.-H., Cheong, S.-W., Park, J.-H., Batista, C. D., & Christianson, A. D. (2021). Decay and renormalization of a longitudinal mode in a quasi-two-dimensional antiferromagnet. *Nature Communications*, 12(1), 5331-5331. <https://doi.org/10.1038/s41467-021-25591-7>

Legros, A., Zhang, S.-S., Bai, X., **Zhang, H.**, Dun, Z., Phelan, W. A., Batista, C. D., Mourigal, M., & Armitage, N. P. (2021). Observation of 4- and 6-Magnon Bound States in the Spin-Anisotropic Frustrated Antiferromagnet Fel_2 . *Physical Review Letters*, 127(26). <https://doi.org/10.1103/PhysRevLett.127.267201>

Bai, X., Zhang, S.-S., Dun, Z., **Zhang, H.**, Huang, Q., Zhou, H., Stone, M. B., Kolesnikov, A. I., Ye, F., Batista, C. D., & Mourigal, M. (2021). Hybridized quadrupolar excitations in the spin-anisotropic frustrated magnet Fel_2 . *Nature Physics*, 17(4), 467-472. <https://doi.org/10.1038/s41567-020-01110-1>

Ishii, Y., Sala, G., Stone, M. B., Garlea, V. O., Calder, S., Chen, J., Yoshida, H., Fukuoka, S., Yan, J., Dela Cruz, C. R., Du, M.-H., Parker, D. S., **Zhang, H.**, Batista, C. D., Yamaura, K., & Christianson, A. (2021). Magnetic properties of the Shastry-Sutherland lattice material $BaNd_2ZnO_5$. *Physical Review Materials*, 5(6)

King, A., Batista, C. D., Raymond, J., Lanting, T., Ozfidan, I., Poulin-Lamarre, G., **Zhang, H.**, & Amin, M. H. (2021). Quantum Annealing Simulation of Out-of-Equilibrium Magnetization in a Spin-Chain Compound. *PRX Quantum*, 2(3), 030317-. <https://doi.org/10.1103/PRXQuantum.2.030317>



Yi Yang

Yang, Y., Han, D., Gao, Y., Zhang, W., Bunn, J., Payzant, E., Yakovenko, A., Penso, J., & Feng, Z. (2022). Residual stress modeling and advanced diffraction measurements of 347H steel weldments. *PVP2022*, 85608.

StART Publications

John Brantley

Fried, A., Breana, J., Nicholas, J., & **Brantley, J.** (2022). Electroediting of Soft Polymer Backbones. *Journal of the American Chemical Society* 144.20 (2022): 8885–8891. Web.

Sindhu Jagadamma

Neupane, A., Herndon E.M., Whitman, T., Faiia, A.M., & **Jagadamma, S.** (2022). Interactive effect of nitrogen and manganese on plant residue decomposition and carbon distribution in soil. *Soil Science Society of America Meeting*. November 6- 10, Baltimore, MD (Oral Accepted).

Jagadamma, S., Neupane, A., Herndon E.M., Whitman, T., & Faiia, A.M. (2021). Manganese-nitrogen interactive control on organic carbon and nitrogen cycling in agricultural soils, *Soil Science Society of America Meeting*. November 7- 10, Salt Lake City, Utah (Oral Invited).

Neupane, A., Herndon E.M., Whitman, T., Faiia, A.M., & **Jagadamma, S.** (2021). Manganese and nitrogen coupled interaction on plant residue decomposition and soil carbon cycling, *Ecological Society of America Meeting*. August 2- 6 (Oral Virtual).

Jian Liu

Meerza, S., Li, Z., Liu, L., Zhang, J., & **Liu, J.** (2022). Fair and Privacy-Preserving Alzheimer's Disease Diagnosis Based on Spontaneous Speech Analysis via Federated Learning, in *Proceedings of the 44th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC 2022)*, Glasgow, Scotland, UK July 2022.

Cui, Y., Li, Z., Liu, L., Zhang, J., & **Liu, J.** (2022). Privacy-preserving Speech-based Depression Diagnosis via Federated Learning, in *Proceedings of the 44th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC 2022)*, Glasgow, Scotland, UK, July 2022.

Li, Z., Zhang, Z., Liu, L., & **Liu, J.** (2022). Auditing Privacy Defenses in Federated Learning via Generative Gradient Leakage, in *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR 2022)*, New Orleans, Louisiana, June 2022.

Li, Z., Liu, L., Zhang, J., & **Liu, J.** (2021). Byzantine-robust Federated Learning through Spatial-temporal Analysis of Local Model Updates, in *Proceedings of the 27th IEEE International Conference on Parallel and Distributed Systems (ICPADS 2021)*, Beijing, China, December 2021.

JDRD Publications

Shuai Li

Cai, J., **Li, S.**, Hu, D., Xu, Y., & He, Q. (2022). Nationwide Assessment of Energy Costs and Policies to Limit Airborne Infection Risks in U.S. Schools. *Journal of Building Engineering*, 103533.

Xu, Y., Cai, J., **Li, S.**, He, Q., & Zhu, S. (2021). Airborne infection risks of SARS-CoV-2 in US schools and impacts of different intervention strategies. *Sustainable Cities and Society*, 103188.

Cao, J., Yang, L., Swanson, C. S., **Li, S.**, & He, Q. (2021). Comparative analysis of impact of human occupancy on indoor microbiomes. *Frontiers of Environmental Science & Engineering*, 15(5), 1-10.

Li, S., Yang, Z., Hu, D., Cao, L., & He, Q. (2021). Understanding building-occupant-microbiome interactions toward healthy built environments: A review. *Frontiers of environmental science & engineering*, 15(4), 1-18.

Xu, Y., Zhu, S., Cai, J., **Li, S.**, & He, Q. (2022). Assessing Transmission Risks of SARS-CoV-2 Omicron Variant in U.S. School Facilities and Mitigation Measures. *Proceedings of the 2022 Winter Simulation Conference*, Accepted.

Schedule 7

CENTERS OF EXCELLENCE ACTUAL, PROPOSED, & REQUESTED BUDGET

Institution: The University of Tennessee

Center: The Science Alliance

	FY 2021-22 Actual			FY 2022-23 Proposed			FY 2023-24 Requested		
	Matching	Appropriation	Total	Matching	Appropriation	Total	Matching	Appropriation	Total
Expenditures									
Salaries									
Faculty	\$616,715	\$447,608	\$1,064,323	\$635,216	\$461,037	\$1,096,253	\$666,977	\$484,088	\$1,151,066
Other Professional	\$126,207	\$329,715	\$455,923	\$129,994	\$339,607	\$469,601	\$136,493	\$356,587	\$493,081
Clerical/ Supporting	\$11,048	\$100,799	\$111,847	\$11,380	\$103,823	\$115,203	\$11,949	\$109,014	\$120,963
Assistantships	\$291,123	\$1,611,478	\$1,902,600	\$299,856	\$1,659,822	\$1,959,678	\$314,849	\$1,742,813	\$2,057,662
Total Salaries	\$1,045,093	\$2,489,600	\$3,534,694	\$1,076,446	\$2,564,288	\$3,640,735	\$1,130,269	\$2,692,503	\$3,822,771
Longevity (Excluded from Salaries)	\$4,024	\$2,545	\$6,569	\$4,145	\$2,621	\$6,766	\$4,352	\$2,752	\$7,105
Fringe Benefits	\$204,071	\$353,039	\$557,110	\$210,193	\$363,630	\$573,823	\$220,703	\$381,812	\$602,514
Total Personnel	\$1,253,189	\$2,845,185	\$4,098,373	\$1,290,784	\$2,930,540	\$4,221,324	\$1,355,324	\$3,077,067	\$4,432,391
Non-Personnel									
Travel	\$21,889	\$31,779	\$53,668	\$22,600	\$100,000	\$122,600	\$25,000	\$55,544	\$80,544
Books & Journals	\$2,307	\$2,380	\$4,687	\$2,382	\$5,600	\$7,982	\$2,532	\$5,064	\$7,595
Other Supplies	\$18,358	\$85,115	\$103,473	\$18,955	\$250,000	\$268,955	\$20,000	\$75,000	\$95,000
Equipment	\$2,479,326	\$2,514,896	\$4,994,222	\$2,049,723	\$2,600,760	\$4,650,483	\$173,590	\$640,586	\$814,176
Maintenance	\$28,434	\$35,170	\$63,604	\$29,358	\$40,000	\$69,358	\$30,000	\$35,000	\$65,000
Other (Specify):									
Prof Services & Memberships	\$728	\$2,261	\$2,988	\$751	\$3,086	\$3,837	\$1,620	\$3,240	\$4,860
Printing, Duplicating, Binding	\$750	\$91	\$841	\$774	\$94	\$868	\$49	\$99	\$148
Utilities and Fuel		\$406	\$406	\$0	\$511	\$511	\$269	\$537	\$806
Communications	\$1,183	\$776	\$1,959	\$1,221	\$1,519	\$2,740	\$798	\$1,595	\$2,393
Computer Services	\$580	\$348	\$928	\$599	\$719	\$1,318	\$378	\$755	\$1,133
Grants & Subsidies (Student Fees)	\$326,593	\$12,933	\$339,526	\$337,207	\$1,000,000	\$1,337,207	\$350,000	\$350,000	\$700,000
Contractual & Special Services	\$63,594	\$15,035	\$78,629	\$65,661	\$400,000	\$465,661	\$65,000	\$20,000	\$85,000
Insurance, Interest & Bad Debt	\$3,790	\$5,790	\$9,579	\$3,913	\$9,890	\$13,803	\$5,193	\$10,385	\$15,578
Awards - Student Aid	\$11,965	\$380,762	\$392,727	\$12,354	\$393,136	\$405,490	\$13,000		\$13,000
Rentals - Other Equipment		\$200	\$200	\$0	\$207	\$207	\$0		\$0
Other Expenditures	\$59,660	\$1,250	\$60,910	\$61,599	\$2,582	\$64,181	\$100,000	\$10,627	\$110,627
Cost Sharing			\$0	\$300,000	\$657,116	\$957,116	\$50,000	\$100,000	\$150,000
Total Non-Personnel	\$3,019,154	\$3,089,192	\$6,108,346	\$2,907,096	\$5,465,220	\$8,372,316	\$837,427	\$1,308,431	\$2,145,858
GRAND TOTAL	\$4,272,343	\$5,934,376	\$10,206,719	\$4,197,880	\$8,395,760	\$12,593,640	\$2,192,751	\$4,385,498	\$6,578,249
Revenue									
New State Appropriation		\$4,040,907	\$4,040,907		\$4,176,665	\$4,176,665		\$4,385,498	\$4,385,498
Carryover State Appropriation		\$6,112,562	\$6,112,562		\$4,219,095	\$4,219,095			\$0
New Matching Funds	\$4,272,343		\$4,272,343	\$4,197,880		\$4,197,880	\$2,192,751		\$2,192,751
Carryover from Previous Matching Funds									
Total Revenue	\$4,272,343	\$10,153,469	\$14,425,812	\$4,197,880	\$8,395,760	\$12,593,640	\$2,192,751	\$4,385,498	\$6,578,249





**University of Tennessee - Oak Ridge
Innovation Institute**

Oak Ridge National Laboratory
P.O. Box 2008, MS6173
Oak Ridge, Tennessee 37931-6173
(865) 341-6744
scialli.utk.edu
scialli@utk.edu

The University of Tennessee is an EEO/AA/Title VI/Title IX/Section 504/ADA/ADEA institution in the provision of its education and employment programs and services. All qualified applicants will receive equal consideration for employment and admission without regard to race, color, national origin, religion, sex, pregnancy, marital status, sexual orientation, gender identity, age, physical or mental disability, genetic information, veteran status, and parental status. The university name and its indicia within are trademarks of the University of Tennessee. A project of the Office of Research and Engagement.