THE UNIVERSITY OF TENNESSEE
KNOXVILLE

SCIENCE ALLIANCE

2016 2017

ANNUAL REPORT

THEC State Appropriations Request 2018-19

CONTENT

SCIENCE ALLIANCE

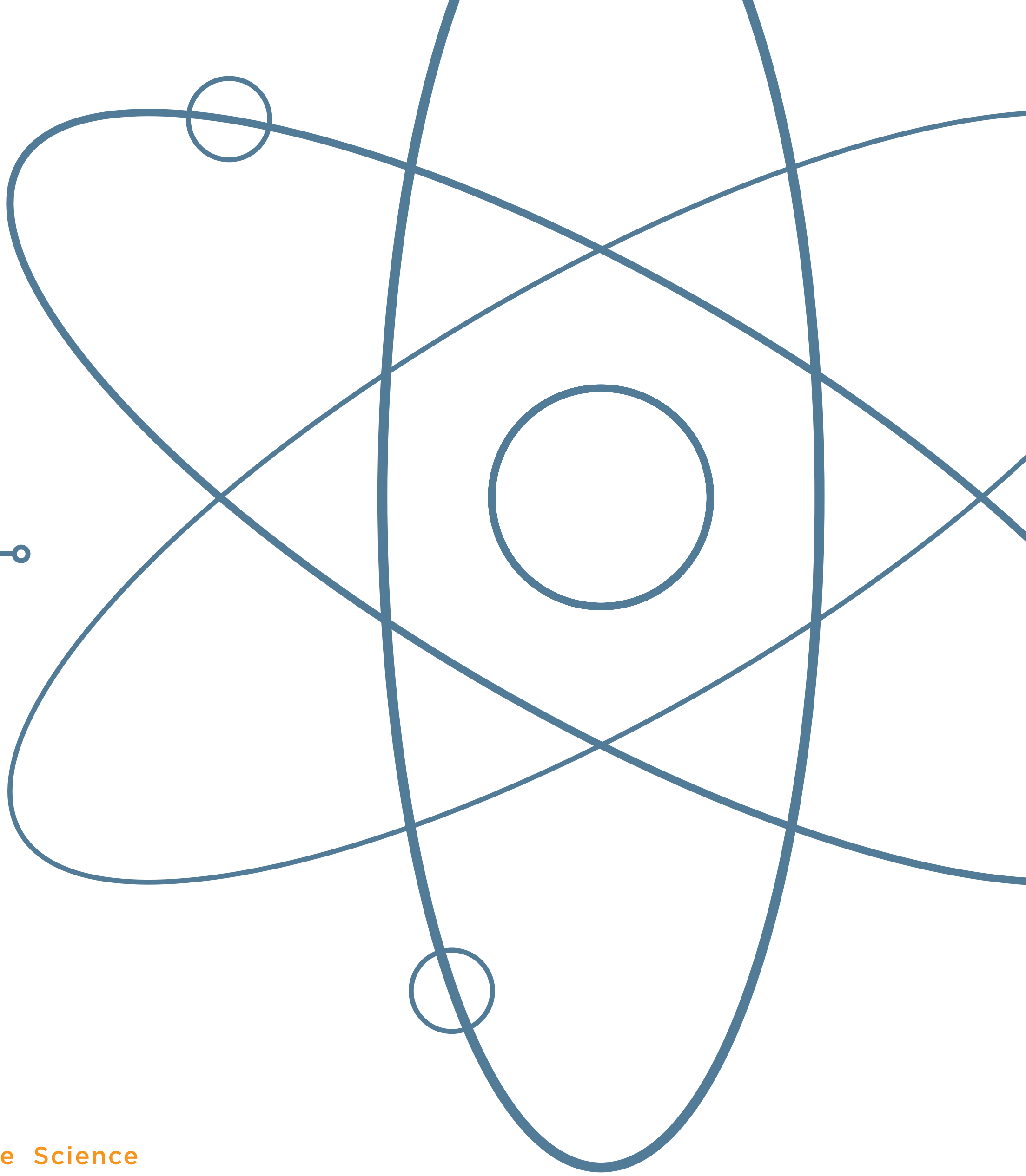
MISSION STATEMENT

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

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

SCIENCE ALLIANCE OBJECTIVES

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



GOALS + FUTURE PLANS

THE PRIMARY MISSION of the Science Alliance has always been to develop and support collaborations between the University of Tennessee and Oak Ridge National Laboratory.

With a solid foundation of decades spent working toward that end, the Science Alliance seeks to amplify that relationship with greater development and educational opportunities. Recent investments in the University-Industry Demonstration Partnership and the Institute for Advanced Composites Manufacturing Innovation have laid the groundwork toward achieving this goal and will help guide the Science Alliance as it develops new cooperative models around stated strategic initiatives. These initiatives will translate into global scientific and economic impacts, intellectual capacity development, and a prepared future workforce for Tennessee.

The Science Alliance will continue to advance these goals by focusing on collaborative strategic initiatives that align around mutual interests, such as exascale computing, data science, and personalized biomedicine. In recent years, the Science Alliance has done this by supporting Joint Directed Research Development projects in these areas as well as investing in the FIRST Robotics Competition, an event designed to motivate high school students to become engaged in STEM fields in a collaborative environment. The co-investment strategies that will support these initiatives will allow the Science Alliance to continue focusing on the joint development and acquisition of talented scientists and engineers as well as continuing to provide consistent graduate student support in areas of global interest.

EXECUTIVE SUMMARY

The Science Alliance continues to be a crucial component in the continued growth of the partnership between the University of Tennessee, Knoxville, and Oak Ridge National Laboratory. Our researchers are collaborating on large initiatives in materials science, biomedical sciences, high-performance computing, and bioenergy science, to name a few.

This spring, UT and ORNL partnered to create a first-of-its-kind data science and engineering doctoral program to meet the needs of a rapidly growing industry: big data. This field has increased in importance across areas ranging from health care to nuclear security. Our students will graduate from this new program with the ability to analyze extremely large data sets to reveal patterns, trends, and associations that could result in life-saving decisions.

Another great collaboration this past year was monitored around the world when a team of scientists from UT, ORNL, and Vanderbilt University helped discover a new super heavy element, Tennessine. Robert Grzywacz, physics professor and director of the UT-ORNL Joint Institute for Nuclear Physics and Applications, helped develop a process that measures the decay of nuclear materials down to one-millionth of a second, which was vital in proving the existence of the new element.

Innovative ideas like these bring competitive faculty members and researchers and attract the highest-caliber students to our university.

More than 140 graduate students received support through the Science Alliance in the past year. Many of them authored publications, presented their research at meetings or conferences, or worked on sponsored projects. These students are working in the nation's leading scientific laboratories and learning how to apply for funding, putting them ahead of their peers.

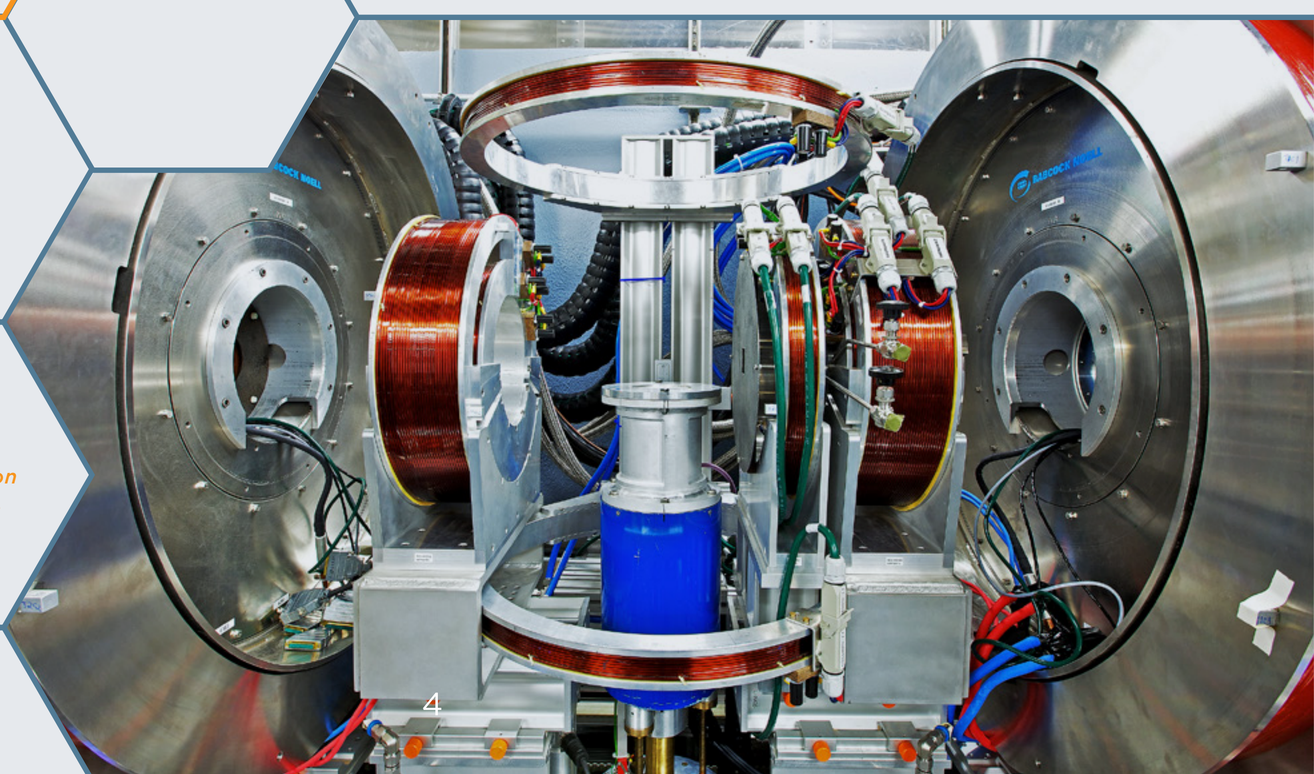
To ensure the success of future scientists and researchers, we must start reaching out to students earlier in their educational careers. That is why the Science Alliance supports FIRST Robotics. The values espoused by FIRST support collaborative research, increased enrollment in higher education, and participation in STEM fields. You will read more about our investment in FIRST Robotics later in this report.

This report is not only a summary of the past year's efforts by our distinguished scientists, Joint Directed Research Development fellows, project leaders, and team members to advance the research enterprise here at UT and with our partners at ORNL, but also a glimpse into the future of research innovation in our nation.

ROBERT NOBLES
Interim Vice Chancellor for Research and Engagement

The strong partnership between the Laboratory and the University continues to produce valuable results for both institutions and for the State of Tennessee. The Science Alliance plays a vital role in sustaining and extending this strategic relationship. I look forward to new opportunities to focus our shared resources on the solution of compelling scientific and technical problems.

THOMAS ZACHARIA
ORNL Director



Spallation Neutron Source at ORNL

UT-ORNL GROWING TOGETHER: A HISTORY OF COLLABORATION

Since the end of World War II, the University of Tennessee and Oak Ridge National Laboratory have been working toward a collaborative relationship. Previously known for its literary, humanities, and agricultural offerings, the university added PhD programs in physics and chemistry in response to increasing demand from Oak Ridge employees and returning soldiers.

In 1964, the university won a Ford Foundation grant that provided the opportunity for national lab scientists to devote some time to teaching at UT. Many UT science faculty members also worked at Oak Ridge as consultants one day a week and over summers.

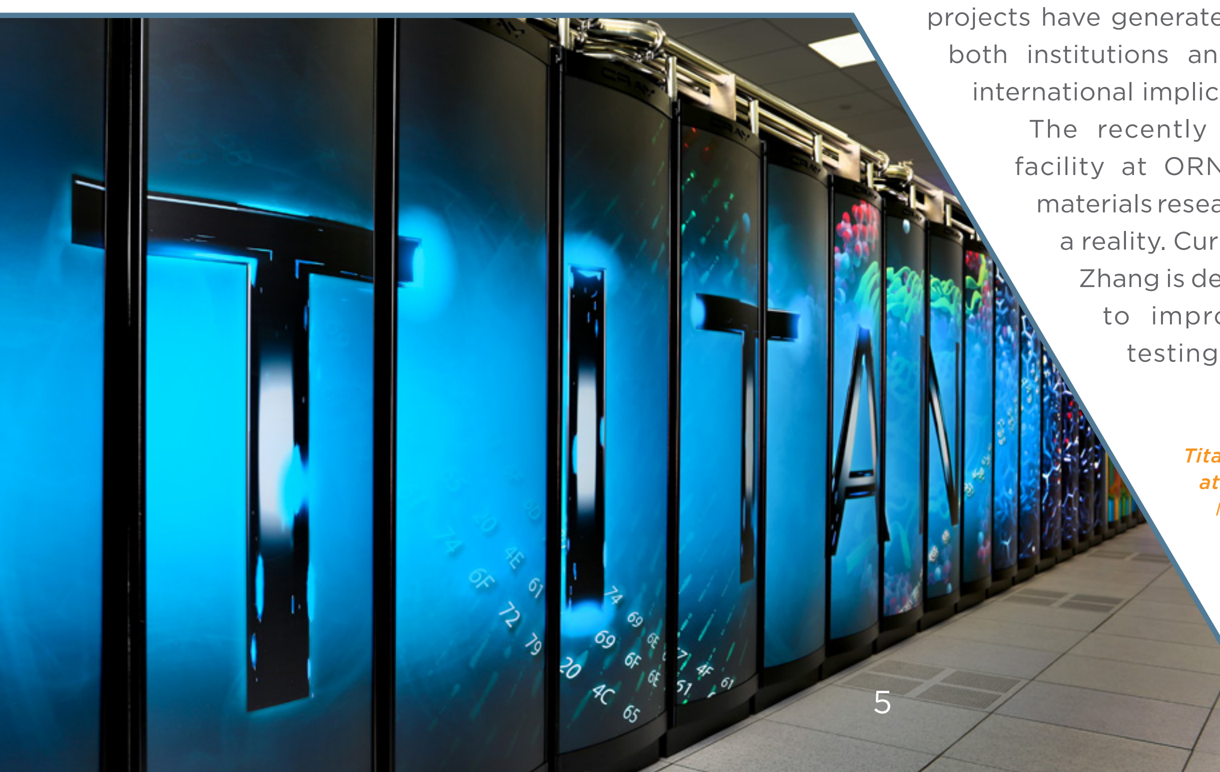
In October 1982, three men sat around a kitchen table in Knoxville and changed the face of UT-ORNL interactions. From this conversation the Distinguished Scientist program and the Science Alliance were born, creating a new model for partnerships between the university and the national lab and laying the foundation for future collaborative efforts, including the joint institutes and UT-Battelle.

"Because of the Science Alliance, because of the joint hires, because of the joint institutes — we were ready to demonstrate the capability to compete," said Lee Riedinger, former interim vice chancellor for research at UT and current director of the UT-ORNL Bredesen Center for Interdisciplinary Research and Graduate Education.

The Distinguished Scientist program was designed to attract high-caliber international researchers to the area and has served as the Science Alliance's anchor program and bedrock to the growing catalog of UT-ORNL collaborations.

The modern partnership between the Science Alliance and ORNL, which still includes the Distinguished Scientist program, has expanded to include the Joint Directed Research Development (JDRD) program now funding 10 to 12 collaborations between UT and ORNL scientists each year. These projects have generated additional funding for both institutions and produced work with international implications.

The recently launched Proto-MPEX facility at ORNL was created to use materials research to make fusion power a reality. Current JDRD recipient Zhili Zhang is developing new algorithms to improve the Proto-MPEX's testing capabilities. Designed



Titan supercomputer built by Cray at Oak Ridge National Laboratory
Images courtesy of the Oak Ridge National Laboratory, U.S. Dept. of Energy.

Workers used a long rod to push uranium slugs into the concrete loading face of the Graphite Reactor at Oak Ridge National Laboratory. Its job was to show that plutonium could be extracted from irradiated uranium slugs, and its first major challenge was to produce a self-sustaining chain reaction.

to investigate fusion plasma and materials that have been exposed to plasma, the Proto-MPEX will likely test materials that will later be used by the International Thermonuclear Experimental Reactor (ITER), the largest multinational fusion experiment in the world.

The partnership between the Science Alliance and ORNL continues to be mutually beneficial. The facilities at Oak Ridge are in high demand, and scientists around the globe jockey for time with neutron beams and supercomputers. By participating in joint UT-ORNL projects, graduate students at the University of Tennessee are uniquely positioned not only to gain experience at a national lab but also to work with equipment unavailable to many investigators in their field.

In return, ORNL researchers gain research partners and extra hands. Current JDRD recipient Maik Lang's graduate students are a prime example of this mutually beneficial undertaking. In addition to having the opportunity to work in a world-class facility, his students will collaborate with ORNL scientists on writing the instructional manual for the modeling system the teams are creating.

As the relationship between the Science Alliance and ORNL continues to grow, the importance of industry involvement in research is becoming more apparent to universities and labs across the country. To that end, UT and ORNL have worked together to develop partnerships with industry leaders such as Goodyear, Cisco, and Boeing. Just last year the Boeing collaboration yielded a Guinness World Records title for the largest solid 3D-printed item, a tool used in manufacturing the Boeing 777X passenger jet.

To continue developing these partnerships, UT and ORNL have co-hosted meetings of both the University-Industry Demonstration Partnership and the Southeast Regional Energy Innovation Workshop. Both events had a similar goal: to improve relationships between industries and researchers in much the same way the Science Alliance cemented the relationship between UT and ORNL. These collaborations will result in positive outcomes for all partnering organizations and the region as a whole.

"The nexus of public-private partnerships involving the deep collaboration between federal government, national labs, industry, and universities is the best way to accelerate innovation and to keep the innovation in the region," said Taylor Eighmy, UT's vice chancellor for research and engagement.

The partnership between the Science Alliance and ORNL has continued to deepen as the two institutions evolve and invest in their futures. UT has just completed construction of Strong Hall, a facility designed to house biology and chemistry teaching labs, and is well on its way to becoming one of the top 25 research universities in the country. ORNL recently completed a review by the US Department of Energy to finalize plans for expanding the existing Spallation Neutron Source facilities, a project that will increase equipment availability and open alternate areas for neutron research.

In the 35 years since that momentous conversation at a kitchen table, the Science Alliance and Oak Ridge National Laboratory have found success and growth in collaboration. Moving forward, the two institutions will seek to develop new collaborative models around shared strategic initiatives, creating more unparalleled opportunities for future generations of educators and innovators. ●

Our partnership with Oak Ridge National Laboratory not only puts UT in elite company nationally, it has a profound impact on the state, the nation, and the world.

JOE DIPIETRO
UT President

IACMI — THE COMPOSITES INSTITUTE

UT, IACMI, Local Motors and ORNL partner to develop 3-D printed composite materials for automotive manufacturing. *Courtesy of Local Motors*

In January of 2015 the University of Tennessee was named the lead institution of the newly formed Institute for Advanced Composites Manufacturing Innovation (now named IACMI — The Composites Institute). Focused on the advancement of composites manufacturing, IACMI is tasked with growing research in the use of composites in a variety of areas, including automobiles, wind turbines, and compressed gas storage tanks. The Science Alliance continued to support IACMI in fiscal year 2017 with $400,000.

Since its creation, IACMI has sought to push the envelope in composites manufacturing. Member institutions have announced partnerships with industry leaders across the globe, from LeMond Composites to DuPont.

In the past year, UT and ORNL have announced two major partnerships through IACMI. Local Motors, one of these partners, is a technology company that designs, builds, and sells vehicles. This collaboration aims to integrate design and materials selection and to discover low-cost reinforcing techniques.

"The integration of design within the materials selection and manufacture process optimizes vehicle production by reducing cycle time," said Gregory Hay, general manager of Local Motors. "The partnership with IACMI — The Composites Institute and its vast group of partners provides access to unique research and development capabilities, ultimately resulting in a more efficient manufacture process for our organization."

In addition to the Local Motors partnership, UT and ORNL have joined with Materials Innovation Technologies (MIT) to create preforms made from recycled carbon fibers. This project is expected to generate outcomes that could save as much as 50 to 75 percent in manufacturing costs.

"The diverse capabilities of IACMI — The Composites Institute and its partners, Oak Ridge National Laboratory and the University of Tennessee, Knoxville, allowed us to work full circle by utilizing reclaimed carbon fiber in the tooling and preforms to produce a lightweight automotive part," said Jim Stike, MIT's president and CEO. "Combining reclaimed carbon fiber with 3D printing processes will greatly reduce the manufacturing time and cost, demonstrating the viability of composite parts in vehicle lightweighting."

IACMI members across the country are reaping the rewards of these university-lab-industry partnerships as composites projects begin to yield tangible results. By leveraging its vast network of collaborators, IACMI is poised to revolutionize the future of composites and additive manufacturing.

"The Composites Institute's impact is larger than the project research and development work taking place at our facilities. Collaboration amongst IACMI members spans the entire industry supply chain," said Byran Dods, IACMI CEO. "Commercialization of new innovations is resulting in the creation of new jobs, expansion of manufacturing facilities, and an overall economic development impact benefiting the entire ecosystem of composites manufacturing." ●

Members of the Farragut team Flagship Robotics celebrate their victory at the 2017 Smoky Mountain Regional FIRST Robotics competition.
Robotics photos by Michael Messing

FIRST ROBOTICS

For Inspiration and Recognition of Science and Technology, or FIRST, was founded in 1989 as a non-profit organization devoted to encouraging young people to participate in science and technology. FIRST's programmatic activities include Lego League, Lego League Jr, and Tech Challenge, but the organization is most readily recognized for its international Robotics Competition.

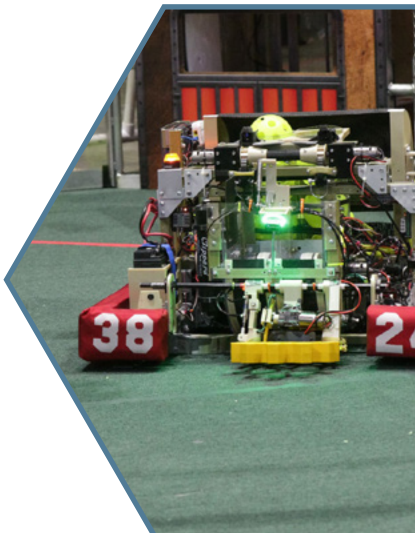
This year's competition presented a challenge requiring competitors to form an alliance with two other teams. Entitled "Steamworks," the task for competitors required the design and construction of robots capable of grabbing and transporting items from one location to another and the ability to climb into the "airship" once challenges were completed.

Robots were also required to operate autonomously from a set of pre-programmed instructions for the first 15 seconds of the competition, leaving two minutes and 15 seconds for operator controlled activity.

For less than three minutes, teams gathered on the floor of Thompson-Boling Arena at the University of Tennessee to compete, working with students outside their own team in an effort to advance to the next round of competition.

The robotics competition is a perfect model of FIRST's core value of "gracious professionalism." Gracious professionalism is the notion that students can learn and compete with one another fiercely, while still treating one another with respect. In addition to nurturing the next generation of scientists, FIRST's practices and values engender the characteristics that make good collaborators.

Collaboration between researchers is the bedrock of the Science Alliance's programmatic activities. For the last two years the Science Alliance has provided support to the Smoky



Mountain Regional FIRST Robotics Competition as a means to foster the future of collaboration in East Tennessee and encourage student participation in STEM fields.

This year's competition included 26 teams from the state of Tennessee, more than any other state participating in the region. At the end of the day, a three team alliance of students from Tennessee, Ohio and Florida had the highest score and will advance to the next round of competition.

The impact of the FIRST Robotics program is undeniable, with research showing 88 percent of participants are more interested in doing well in school. Additionally, more than 75 percent of FIRST Robotics alumni are either students or professionals in a STEM field.

The Science Alliance's activities encourage collaboration as a model for future innovation in research. The work of FIRST and the FIRST Robotics Competition, by laying the groundwork for a future generation of collaborators, is a natural step toward that model for innovation. Providing support to the FIRST organization helps offer a wealth of opportunities to young students in the state of Tennessee and contributes directly to the future of innovation and research.

DISTINGUISHED SCIENTISTS

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

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

In the future, we intend to explore Distinguished Scientist positions that are co-supported by endowments from our corporate research and development partners. This structure may allow us to amplify the investments made by the state and ORNL in areas of interest to our key industrial research and development partners.

ELBIO DAGOTTO Elbio Dagotto primarily uses computational techniques to study transition metal oxides, oxide interfaces, and the recently discovered iron-base high-temperature superconductors. These materials, and others studied by his group, show promise for both technological applications and advancement of fundamental concepts in condensed matter physics. Dagotto has several active collaborations with ORNL scientists working with materials from manganese oxides to iron-based high-temperature superconductors. Additionally, he serves as principal investigator of a US Department of Energy field work proposal, Theoretical Studies of Complex Collective Phenomena, which secured a grant from the DOE that awarded $1,992,999 over eighteen months to ORNL.

TAKESHI EGAMI The physics of liquids is much less developed than the physics of solids. Takeshi Egami explores liquids and gases using computer sim-ulation, including quantum mechanical calculations, and neutron and synchrotron x-ray scattering experiments. Egami is currently parti-cipating in a number of active collaborations with ORNL scientists, including DOE projects whose fiscal year budgets total more than $2.7 million. Egami was recently named an Aris Phillips Lecturer by Yale University, the most prestigious award given by their Department of Mechanical Engineering. Additionally, Egami has served as editor for *Advances in Physics* since 2011 and as divisional associate editor in condensed matter physics for *Physical Review Letters*.

BOB HATCHER A structural and tectonics geologist, Bob Hatcher studies the processes that create and evolve Earth's continental crust. His team conducts detailed field and laboratory studies of the Appalachians and other ancient and modern mountain chains worldwide, as well as related studies that try to answer the question of why there are earthquakes in the eastern United States. Hatcher is currently serving as principal investigator on a project, supported by the US Nuclear Regulatory Commission, studying paleoseismology of the East Tennessee seismic zone. His collaborations with scientists at the University of Memphis and the US Geological Survey have yielded important information about seismic hazards in East Tennessee. In 2014 he was the recipient of the Marcus Milling Legendary Geoscientist medal, and he was recognized along with scientists from six other countries at the Geological Society of America Penrose Conference.

DAVID JOY David Joy's research helps create accurate microscopic and nanoscale imaging techniques, including the new, superior helium ion beam microscope which is more flexible and powerful than electron microscopy and could ultimately offer direct, high resolution imaging at subatomic and subnanometric scales. Since its creation, Joy's microscope has been used consistently at ORNL. This instrument joins the Zeiss Transmission Electron Microscope, which Joy was directly responsible for acquiring, to a total benefit in excess of $5 million in microscopy alone. Additionally, Joy serves as member of the editorial board for the *Journal of Microscopy* and is a regular reviewer for a number of major publications, including *Nature Materials*, *Physical Review Letters*, *Journal of Applied Physics*, and *Applied Physics Letters*.

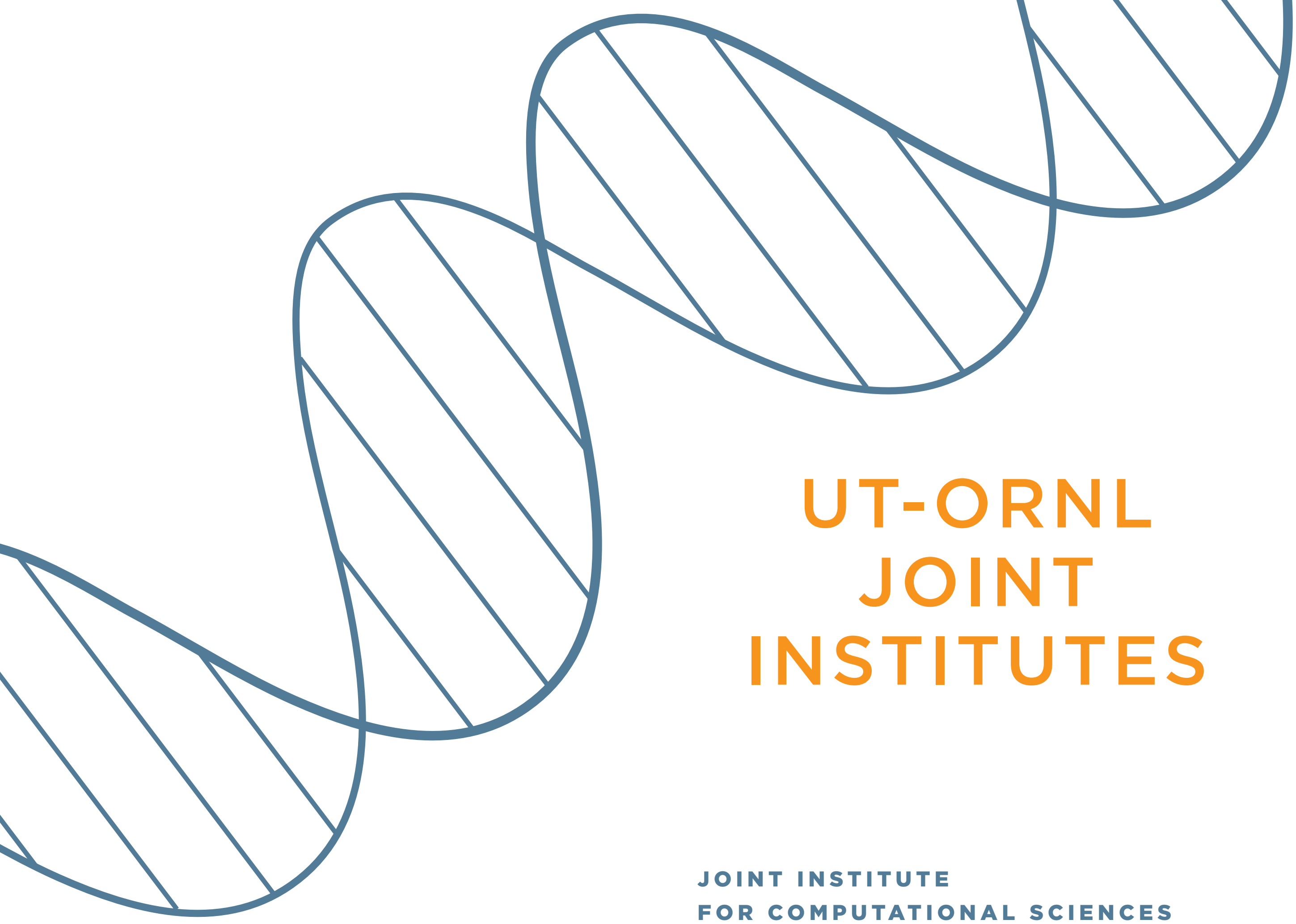
JIMMY MAYS Jimmy Mays synthesizes new, precisely tailored polymers and examines their molecular architecture, composition and blending capability to discover how form and structure, including their nanostructural order, might be manipulated to create useful materials. Currently, Mays is a member of Alexei Sokolov's DOE Field Work Proposal on "Polymer Based Multicomponent Materials," a program funded at $2 million annually that Mays led prior to Sokolov's arrival. Addtionally, he is serving as Co-Principal Investigator on several ORNL based polymer projects. In 2014, Mays was named a Fellow in the Royal Society of Chemistry, as well as Guest Professor at Soochow University in Suzhou, Cina.

CLAYTON WEBSTER Clayton Webster's research interests include approximation theory, numerical and functional analysis, as well as high performing algorithms, with particular focus on large-scale applications. Webster is the department head in the Department of Computation and Applied Mathematics at ORNL. In 2007 he was awarded the John von Neumann Fellowship by Sandia National Laboratories. In 2008 he was named the Director of Quantitative Analysis & Trading at NextEra Energy Power Trading, LLC. In 2014 he became a Frontiers of Science Fellow, awarded by the National Academy of Sciences.

FUNDING

PRIN INV.	PROJECT NAME	PROJECT TITLE	START DATE	END DATE	AWARD AMOUNT	FY 17 EXPEN-DITURES
Dagotto	NSF-DMR-1404375	Computational Studies of Multiorbital Model Hamiltonians for Iron-Based Superconductors in Quasi One-Dimensional Geometrics	09/01/14	08/31/17	435,000	117,549
Egami	UT-B 4000126542 Egami	Dynamics of Biologically Relevant Model Membrane Systems	09/20/13	09/30/17	117,337	
Egami	UT-B 4000149639 Egami	Viscosity of Aqueous Solution	08/23/16	07/31/18	144,217	110,502
Egami	UT-B 4000139883 Egami	Neutron Scattering Study of Disordered Materials Under pressure	06/16/15	07/31/17	59,649	42,609
Egami	UT-B 4000119538	Physics of Metallic Glasses	01/01/13	02/28/17	563,546	3,153
Egami	UT-B 4000131427 Egami	Local Structure by Neutron Diffraction	07/01/14	12/29/17	180,000	10,974
Egami	UT-B 4000131427 Egami (Year 2)	Local Structure by Neutron Diffraction	07/01/15	12/29/17	241,949	149,051
Egami	UT-B 4000139883 Egami	Neutron Scattering Study of disordered materials under pressure	06/16/15	07/31/17	58,099	4,436
Egami	UT-B 4000120790 Egami	Atomistic Study of Bulk Metallic Glasses	03/15/13	12/31/17	425,021	1,010
Egami	Carnegie Inst of Was 4-10114-12 Egami	Study of Conducting Oxides Under pressure	03/01/16	07/31/17	162,606	149,168

PRIN INV.	PROJECT NAME	PROJECT TITLE	START DATE	END DATE	AWARD AMOUNT	FY 17 EXPEN-DITURES
Hatcher	NRC-HQ-11-G-04-0085-Hatcher	Two-Year Collaborative Research Project to Assess Large Earthquake Seismology in the ETSZ	09/26/11	09/25/16	454,706	31,139
Hatcher	USDI-NPS P15AS01406-Hatcher	New Geological Map of Chickamauga & Chattanooga National Military Park	08/31/15	10/31/16	43,000	2,577
Hatcher	USGS G16AC00138-Hatcher	Geologic mapping of the Parksville 7.5-min quadrangle, & the kinematics of emplacement of larger horses along a major thrust fault, southeastern Tennessee	05/01/16	09/30/17	17,500	13,382
Mays	Dow Chemical Co. Jimmy Mays	Unrestricted Research Support	10/30/02	12/31/47	35,000	193
Mays	Vanderbilt Univ Sub No. 2016-015735	Improved Carbon Nanotube Fibers through Crosslinking & Densification	01/01/13	12/31/16	371,250	12,388
Mays	UT-B 4000152655	Designing the next generation high performance polymeric cathodes	01/19/17	09/30/17	20,000	20,496
Mays	UT-B 4000152999	Polymer Synthesis	02/06/17	05/31/17	20,546	20,549
Mays	UT-B 4000153000	Scaled-up synthesis of deuterated isoprene	02/15/17	08/13/17	20,000	16,075
Mays	NOVA Chemicals Well-Defined Long	Well Defined Long Chain Branched Polythylene by Living Anionic Polymerization of 1,3-Butadiene & Hydrogenation	10/19/16	12/31/17	170,012	145,949
Webster	NSF DMS-1620280	Collaborative research: Mathematical methods for approximation & control of multi-dimensional parameterized systems	09/15/16	08/31/19	65,752	



UT-ORNL JOINT INSTITUTES

JOINT INSTITUTE FOR ADVANCED MATERIALS

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

JOINT INSTITUTE FOR BIOLOGICAL SCIENCES

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

JOINT INSTITUTE FOR COMPUTATIONAL SCIENCES

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

JOINT INSTITUTE FOR NUCLEAR PHYSICS AND APPLICATIONS

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

SHULL WOLLAN CENTER, A JOINT INSTITUTE FOR NEUTRON SCIENCES

The Shull Wollan Center promotes world-wide neutron scattering collaboration among researchers in biological and life sciences, energy sciences, polymer science, condensed matter physics, and computational sciences. ●

JOINT DIRECTED RESEARCH DEVELOPMENT

The Joint Directed Research Development (JDRD) program offers an opportunity for collaborative research with ORNL.

A dual UT and ORNL venture, JDRD complements the Laboratory Directed Research Development (LDRD) program and ORNL Seed Money Fund. The LDRD is a US Department of Energy program that encourages multi-program DOE laboratories such as ORNL to select a limited number of projects with the potential to position the lab for scientific and technical leadership in future national initiatives.

The ORNL Seed Money Fund provides a source of funding for innovative ideas that have the potential to enhance the laboratory's core scientific and technical competencies and provide a path for funding new approaches that fall within the distinctive capabilities of ORNL but outside the more focused research priorities of the existing major initiatives. The JDRD program identifies and supports corresponding areas of research at UT, and projects approved for the program have both a UT and ORNL component.

JDRD awards 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 the partnership development research progress thus far.

CHRISTOPHER BAKER

Biofuel is not a new product. When the first diesel engine was presented at the World Exhibition of Paris in 1900, it ran on peanut oil. Henry Ford's Model T was designed to use hemp-derived biofuel, and even ethanol was in use during World Wars I and II. The past 20 years have seen a resurgence in interest and research pertaining to biofuels as scientists venture beyond corn-based ethanol.

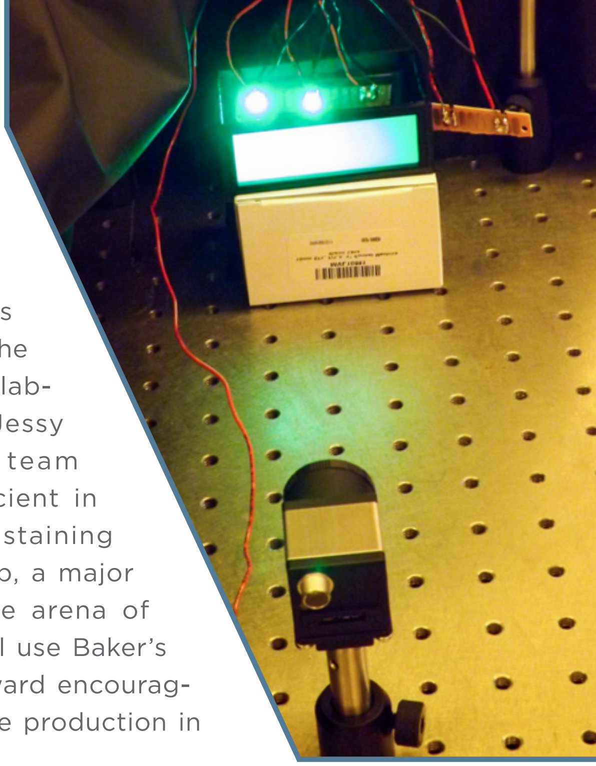
"Most gasoline is about 10 percent ethanol," said Christopher Baker, assistant professor of chemistry. "The problem is that to produce ethanol we have to feed other types of cells — yeast for example — these refined sugars. The effort it takes to produce that sugar is more energy than we get back out when we produce the ethanol."

Baker's JDRD project is an early step toward finding alternatives to this expensive fuel-making process by studying fungi. Fungi have evolved over millions of years to survive in challenging environments, in part through their ability to find nutrients where other types of cells cannot. One of the ways they do this is by secreting a chemical that helps digest otherwise indigestible substances.

Fungi can often be seen growing on tree bark — but how are they surviving there? Tree bark is generally composed of lignocellulose, a polymer network of sugar molecules. Because they are linked, these sugars can't be used as nutrients. This is where the fungi come in. They produce an enzyme called laccase that pulls the lignocellulose apart, breaking it down into its base sugars. Those sugars can then be used to make fuel.

"Once you can take these materials that are otherwise not nutrients and turn them into nutrients, you can feed those nutrients to something like a yeast cell and the yeast cell will turn that sugar into alcohol. That's a vital, important step for producing biofuels," said Baker.

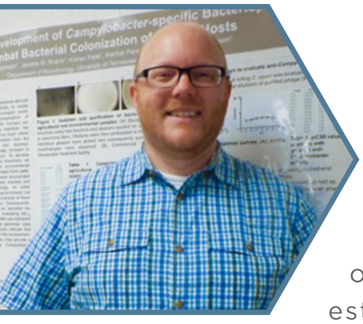
Baker's JDRD team is building a sensor platform designed to study laccase secretion. His platform will allow for the rapid high-throughput study of the effect of a variety of reagents on fungal cells with reference to enzyme production.



Once the platform is complete, Baker's team will hand off the device to their collaborator at ORNL, Jessy Labbé. Labbé's team has become proficient in producing and sustaining fungal cells in a lab, a major achievement in the arena of mycology. They will use Baker's device to work toward encouraging the best laccase production in their fungal cells.

"They have this unique ability to genetically engineer fungi," said Baker. "Our technology will allow them to make many genetic modifications, screen them all in this high-density platform, and be able to see which is producing the most of this enzyme."

Baker's project not only will improve biofuel production, but also — because fungi are important in medicine, agriculture, and basic biological research — has the potential to affect a number of vital research areas. ●



JEREMIAH JOHNSON

In 2010, over the course of seven months, an outbreak of *Salmonella* caused an estimated 1,939 cases of food poisoning across 11 states, including Tennessee. The US Centers for Disease Control (CDC) launched an investigation to trace the source of the infections, which was ultimately attributed to eggs from two distributors in Iowa. The CDC investigation was successful due to DNA testing of the specific strains of *Salmonella* causing the epidemic. This testing allowed the CDC to locate the source of the infection and prevent further spread of the epidemic by encouraging a recall of the contaminated eggs. Such effective techniques, however, are not widely available for another source of foodborne illness, *Campylobacter*. Jeremiah Johnson, assistant professor of microbiology, and his JDRD team plan to change that.

"*Campylobacter* recently became the most common cause of foodborne bacterial infection in the United States," said Johnson. "It is thought that most people get it from eating contaminated undercooked chicken, because birds carry it within their digestive tract —*Campylobacter* is to chickens what *E. coli* is to cattle. Unfortunately, there's not a lot of data that chickens are the primary cause of *Campylobacter* infection in humans, and it remains mostly circumstantial."

According to Johnson, this information gap for *Campylobacter* results from the use of older techniques, such as pulse-field gel electrophoresis, which can look only at coarse differences in the genomes of bacterial strains. This has been effective for studying *E. coli* and *Salmonella* transmission, but *Campylobacter* is unique in that its genome changes very rapidly, making it difficult to trace back to a source. To combat this challenge, state public health departments have received directives to start using whole-genome sequencing in an attempt to locate the sources of the infections.

"Unfortunately, a lot of the public health departments don't have that know-how yet. They're acquiring the sequencing machines, but they don't have the bioinformatics expertise needed to analyze those genomes. That's where we come in," said Johnson.

Johnson's JDRD team is working with *Campylobacter* strains isolated across East Tennessee, including those collected by the US Food and Drug Administration and the Tennessee Department of Health, to conduct an in-depth analysis of the bacterium's genome. Once the analysis is complete, Johnson hopes it will lead to a better understanding of the bacterium, as well as discovering why East Tennessee has the highest rate of *Campylobacter* infection in the state.

"The Department of Health suspects that it's not entirely linked to chicken consumption. They don't really know where it's coming from. Because of our experience with whole-genome sequencing, they're thinking that we can take our expertise, the expertise at ORNL, and try to find out where some of these infections are coming from," said Johnson.

Dan Jacobson, Johnson's ORNL partner and a computational biologist, will use the information generated by the JDRD team to conduct a broad analysis of the *Campylobacter* genome. Given the rate at which *Campylobacter*'s genome changes, this evolutionary view should aid in tracing strains back to their origination point. ●

VEERLE KEPPENS

Within the past 20 years, portable devices such as mobile phones and laptop computers have become increasingly important parts of everyday life. The ability to carry such devices from place to place has revolutionized communication, academic study, project management, and more. That technology exists largely due to the transistor.

Transistors are essentially switches that turn on and off depending on the function being performed. Typically made with semiconductors, transistors are steadily becoming problematic as scientists approach the limit of how small they can be made while still maintaining effectiveness. This is where Veerle Keppens, director of the UT-ORNL Joint Institute for Advanced Materials and head of the materials science and engineering department in UT's Tickle College of Engineering, and graduate student Amanda Haglund step in.

"I'm trying to grow materials that were first discovered in the 1960s but have not received much attention since," said Haglund. "They're semiconductors and they're magnetic at the same time. With these, if we can make magnetic-based transistors they could switch faster than the existing semiconductors."

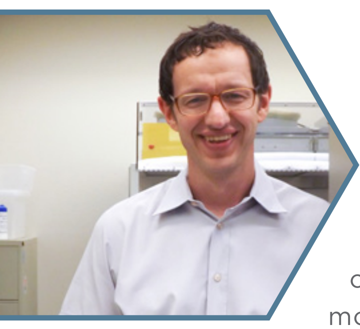
According to Keppens, these transistors would be more efficient and able to continue decreasing in size. In its second year, Keppens's JDRD project has had some success growing crystals uncovered by Haglund's research. For the remainder of the year, the team plans to continue pulling materials from the history books.

"I'm still trying to find new ones to grow. When you look at the elements in a compound, you see that you should be able to grow a new material by replacing some of its constituents with elements that have similar properties. But nobody's done it yet, so there are a few that I'm trying to figure out how to get them to grow," said Haglund.

Keppens's goal is to close the final year of this JDRD project with a strong proof of concept she can then leverage to bring larger grants into the university.

"A lot of times NSF [the National Science Foundation] and DOD [the US Department of Defense] want some results, something that shows you can actually do what you're saying you can do, that it's something you have expertise in so you can expand on it with bigger federal funding grants," said Keppens.

Keppens's team is working in parallel with their ORNL partner, staff scientist Thomas Ward, in an emerging research area. According to Ward, the collaboration between these two projects has the potential to place UT and ORNL as leaders in the field as it continues to develop. ●



MAIK LANG

The Spallation Neutron Source (SNS) at ORNL is a unique research facility capable of producing the most intense neutron beams currently available anywhere in the world. With this beam technology, SNS offers unprecedented research and data collection opportunities through neutron scattering. Unfortunately, that data does not emerge in a readily useful format. Maik Lang, assistant professor of nuclear engineering and Pietro F. Pasqua Fellow, is working to change that.

Lang's JDRD project focuses on understanding the effects of extreme conditions on glass. His team has already gathered initial neutron scattering data that will be used by his ORNL partners to set up a new integrated environment for translating raw data into a usable format.

"This platform will help to process your raw data collected at the spallation source and better understand that data and tie it together to other measurements you did at different beam lines, or even at different facilities," said Lang.

This platform, the Integrated Computational Environment-Modeling and Analysis for Neutrons, or ICE-MAN, will work as a translator, taking the information logged by the SNS and converting it into the format needed for modeling and analysis.

"It's kind of like a black box. The data enters in one format and then the black box changes it into the right format for your software or models," said Lang. By integrating his "black box" with the measuring device, Lang hopes to streamline the process from data collection to useful information for researchers studying a variety of materials.

This technology will allow Lang to use his data to model the effects of radiation on glass, a popular storage substance for nuclear waste. Researchers need to know exactly how and when glass and other storage materials begin to break down from exposure to plasma in order to determine possible uses and future complications.

According to Lang, the disordered nature of glass makes it especially difficult to study, as the effects of radiation are very subtle.

"When you have glass, it's a noncrystalline material so you have no order. When you measure you get a lot of peaks but don't know what it means," said Lang. "You have data but you can't interpret it. For this you need modeling, and for the modeling we need this platform."

Lang's team will assist a team at ORNL led by Anibal Ramirez, chemical spectroscopy group leader, in setting up ICE-MAN using the JDRD project data and in creating a manual for the system. Lang believes this collaboration will not only create opportunities for future efforts and funding but also open the door for discovery in materials science as a whole.

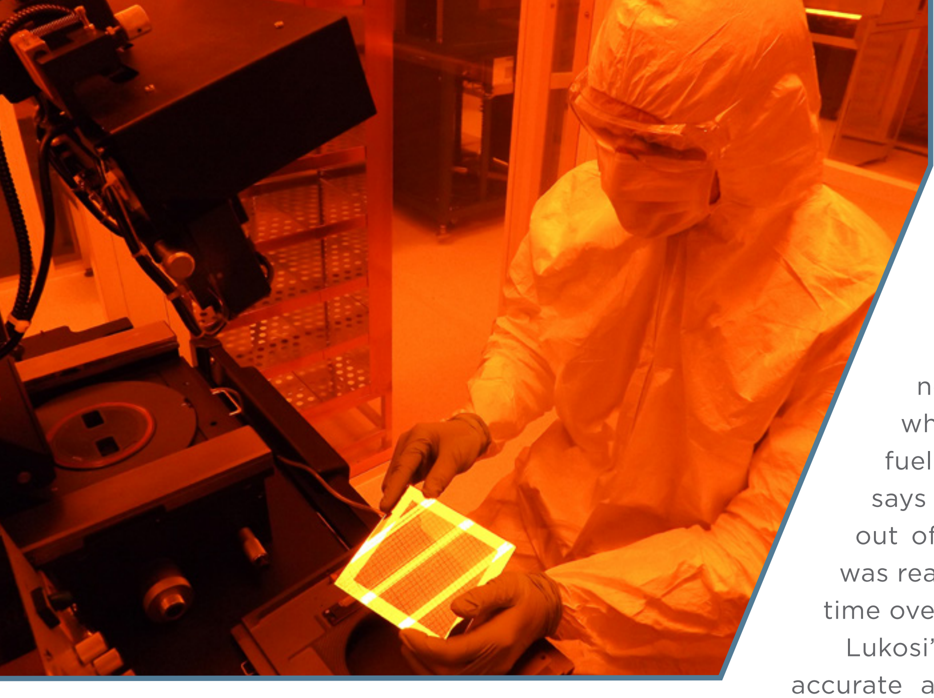
ERIC LUKOSI

According to the National Cancer Institute, approximately 39.6 percent of men and women will be diagnosed with cancer over the course of their lifetime. In the United States cancer is responsible for roughly 171 out of every 100,000 deaths. The number of patients living beyond a cancer diagnosis is on the rise, however, thanks to ever-improving treatments.

Radiation therapy, or radiotherapy, has become increasingly popular, with an estimated 60 percent of cancer patients in the US receiving it at some point. The JDRD team headed by Eric Lukosi, assistant professor of nuclear engineering, proposes to improve those treatments through the creation of a microfluidic device. This device will integrate with the treatment apparatus and measure dosage and purity in addition to removing steps from the measuring process.

"There have been experiments performed using actinium-225 and bismuth-213 that show they are extremely effective at radiotherapy," said Will Gerding, the graduate student supported by Lukosi's JDRD project. "One of the downsides of that is to make sure you have the right ratio you need to do gamma spectroscopy in a separate device. That makes the process a bit longer and causes the bismuth, from radioactive decay, to become less effective."

When actinium decays it eventually becomes bismuth — specifically, the isotope of bismuth needed for radiation treatments. One of the ongoing challenges with these treatments is ensuring that the bismuth is making its way into patients but the actinium is not. Currently, gamma spectroscopy is used to assess the purity of the treatment.



"There is actually a whole host of applications for this technology. I originally thought of the idea for nonproliferation for pyroprocessing, which is electrifying spent nuclear fuels," said Lukosi. "So when someone says he removed two tons of plutonium out of this fuel, how do we know that it was really two tons? Is he taking grams at a time over years to sell to terrorists?"

Lukosi's device would be able to provide accurate and detailed measurements of the contents of the fluids that pass through it. That precision would make it a useful tool for researchers in a number of fields, including medical treatment.

Working with his ORNL partner, Senior Research Scientist David DePaoli, will provide Lukosi an opportunity to test the device on the actinium/bismuth generating system they are building. With positive outcomes, this UT-ORNL partnership could potentially increase the number of patients outliving their cancer diagnoses in future generations. ●

In order to conduct the gamma spectroscopy, the solution must be taken from the dispenser to a different location and processed through multiple steps before being put into a vacuum for the final spectroscopic analysis. The process requires a great deal of time, during which the bismuth may decay past its effective stage before it can be examined.

"If you could just push it through my microfluidic sampler, that would remove a lot of steps there — so it would be a time- and cost-saving measure for radiochemists analyzing samples," said Lukosi.

Lukosi's JDRD work has a host of potential applications, including environmental sampling and nuclear nonproliferation.

SHARANI ROY

The pharmaceutical industry is a multibillion-dollar business that touches the lives of nearly everyone on earth in one way or another. In the United States alone, about four billion individual prescriptions are filled at pharmacies across the country each year. The California Biomedical Research Association estimates that 12 years of development goes into the creation of a single drug. Sharani Roy, assistant professor of chemistry, could impact that development process with her JDRD project.

Surface chemistry — specifically heterogeneous catalysis, the acceleration of a chemical reaction on the surface of a solid — has played a major role in pharmaceutical research for a number of years. Members of Roy's JDRD team have focused their efforts on controlling the outcome of the reaction generated by heterogeneous catalysis, or catalytic selectivity.

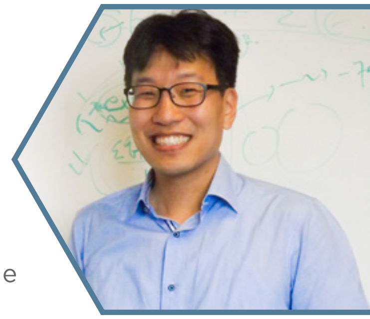
"Two reactants come together. They react, and maybe there are two or three different possible products: A, B, and C. But how do you design a catalyst so that it makes A but not B and C? A lot of times you don't want all the products. You're looking for a particular one," said Roy.

Roy's team will study the process of catalytic selectivity by examining these surface reactions, which she hopes will lead to a better understanding of how to create and control that selectivity. The ability to direct this reaction could play a major role in advancing and expediting pharmaceutical research and drug creation. In the second phase of her project, Roy will study selectivity in a more realistic environment.

"In industry, when people are making a molecule in bulk, you don't have these pristine surfaces that you make in the laboratory," she said. "They are using what they have. They have high-pressure conditions and temperature conditions. Those are the real catalysts that are used every day. There's a gap between that and these very model, ideal systems that we study in the laboratories."

Roy's ORNL partner, research scientist Benjamin Doughty, will provide her team with chemical images captured via the vibrational sum-frequency generation microscope he developed. The two hope their collaborative efforts result in a more complete understanding of interfacial molecular processes. ●

SEUNGHA SHIN



On November 2, 1944, Howard Hughes's infamous plane the *Spruce Goose* made its inaugural and final flight, traveling a single mile. Contrary to its name, the *Spruce Goose* was constructed primarily of laminated birch in an attempt to work within the government's wartime materials restrictions. Weighing approximately 300,000 pounds, the plane was estimated to travel less than a quarter of a mile per gallon of fuel. In contrast, a modern Boeing 747 travels approximately five miles on a gallon.

Aside from the modern technology operating within the 747, the most obvious difference between the two aircraft lies in their construction materials. The 747 is made of a high-tech aluminum alloy. The study and improvement of aluminum alloys continue to make up an important area of research within the field of materials science.

Lighter, more heat-resistant alloys can improve the performance and fuel efficiency of transportation vehicles like cars and planes. This is precisely the subject Seungha Shin, assistant professor of mechanical, aerospace, and biomedical engineering, proposes to address with his JDRD project. Shin's team, in conjunction with his partner Amit Shyam, a research scientist at ORNL, is investigating mass and thermal transport near microstructural interfaces in the search for better-designed aluminum alloys.

"Aluminum is kind of a soft metal, so in order to have better mechanical properties we add copper. In mechanical properties, most failures occur near the interface, so when designing a microstructure, the interface is very important," said Shin.

Shin hopes his project will lead to a more thorough understanding of how to design alloys to create microstructures that provide specific effects, such as greater durability under high temperature conditions.

"Normally, light metals are not that good at high temperatures, so to use that kind of lightweight metal we need to develop some new materials," said Shin.

Microstructures have an important role to play in the development of these new materials. The unique microstructure of a material determines its physical properties, such as toughness, corrosion resistance, and thermal transport behavior. These properties then determine the applications and industries for which that material is suited. Essentially, microstructures dictate the uses of materials.

"If we have an aluminum-copper alloy, it creates a certain phase of microstructure called the theta phase. It begins all mixed together, then forms the theta prime phase followed by the theta phase," said Shin. "The theta phase is not good, but the theta prime phase can create a stronger aluminum alloy. We want to prevent the diffusion, or transition, from the theta prime to theta phase."

Shin's team will focus on computational simulations of interfacial transport at the atomic level with the goal of developing a theoretical framework for controlling these properties. His ORNL partners will model on both fundamental and system scales. Shin's work will provide the missing piece for effective alloy design, with wide-ranging applications in air and ground transportation. ●

OLEG SHYLO

Imagine a busy airport. Planes from a dozen airlines take off and land hundreds of thousands of times a day, heading to and from hundreds of cities. Passengers scurry from plane to plane catching connecting flights to arrive at their final destination. To ensure that the whole system works reliably and efficiently, complex and large-scale decisions have to be made.

In mathematical language, the decision-making process can be formulated as what computer scientists call an optimization problem — one that looks for the best possible solution out of many alternatives. In the airport setting, this approach will ensure that thousands of planes can take off and land in an orderly fashion and relatively on schedule.

Optimization models that fully capture the essence of industrial-scale problems require computational capacities afforded only by high-performance computing systems. Oleg Shylo, assistant professor of industrial and systems engineering, is hoping to utilize these systems in his JDRD work by designing new algorithms to work in parallel.

"The approach that we're taking is so-called cooperative solvers, where a group of optimization algorithms work together and, as the word cooperative implies, they communicate with each other to solve problems," said Shylo.

The use of cooperative solvers comes with its own unique set of constraints, as the communication between these algorithms can quickly overwhelm the system's bandwidth. Optimization problems frequently have a large number of variables and need to be solved very quickly, something that can't happen if algorithms are using all the computing power to share updates.

"As in human communication, if you have 10,000 people talking to each other at the same time it's going to be chaotic and you won't have time to do any useful work," said Shylo. "The same applies to algorithms. You need to design communication structures and topologies to alleviate those kinds of issues."

Shylo will use theoretical models to discover the best communication structures. Through his LDRD partnership with Jack Wells, director of science for the Oak Ridge Leadership Computing Facility at ORNL, Shylo will have the opportunity to test his algorithms on one of the high-performance computing systems, such as Titan, at the national lab. He hopes these tests will confirm his theoretical work and clear the path toward solving real-world optimization problems. ●

HAIXUAN XU

In baking, cooks often start with a simple recipe of flour, baking powder, butter, sugar, and eggs. This basic list of ingredients will come together to make a base for a variety of different goods. From here, the addition of milk will turn that base into cake batter, while baking soda will make cookie dough. The use of different ingredients in the same base can lead to vastly different outcomes.

The same can be said of materials science and the study of low-dimensional materials. Haixuan Xu, assistant professor of materials science and engineering, and his JDRD team propose to expand the understanding of the effect of point defects and impurities on low-dimensional materials such as graphene.

"We are trying to see how we can control the creation of defects in low-dimensional materials," said Xu. "A defect could be a hole or what you call a vacancy in the material system. Then we want to put something else in there. That's called a dopant."

Dopants, or impurities, are inserted into a substance to change its electrical or optical properties. This is often done with semiconductor materials currently of interest in the advancement of electronics and computing.

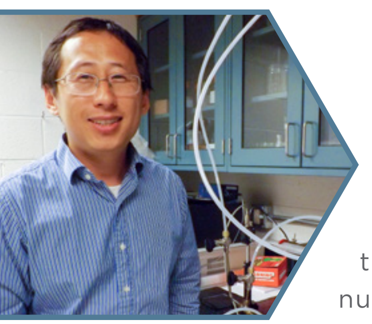
The ultimate aim of Xu's work is to advance the science of quantum computing by contributing to the foundation of knowledge needed in order to move forward.

"The joint LDRD [Laboratory Directed Research and Development] and JDRD work is trying to see if we can precisely control the atomic and material environment used to prepare and maintain coherent superposition of quantum states, which is the heart of the challenge for quantum computing. But there are many steps in between," said Xu.

Xu's project will study these defects in an attempt to ascertain how the use of particular dopants can affect the base material, particularly with relation to the electronic structure of the system. In order to do this, his team must first determine how to create defects in a controlled manner, a task that is currently under way.

Xu's ORNL partner, Stephen Jesse, will tackle the same problem from an experimental angle using the national lab's scanning electron beam microscope and helium ion microscope. Xu's team will be hammering away at the theoretical understanding through computer modeling, with the intention of bringing their results together to provide a more complete picture.

"There is nice synergy between the Oak Ridge and UT teams. We're actually studying the same scientific problem from two different and complementary perspectives," said Xu. "Hopefully we can get a better understanding of what's really going on in the system." ●



ZHILI ZHANG

In the 1920s Arthur Eddington proposed that the process of fusing small nuclei together, or fusion, released large amounts of energy and was in fact what powered the stars. Since that time fusion power has been an important area of study, but despite nearly 100 years of research, controlled fusion remains elusive.

In recent years, the plasma-wall interaction within fusion devices has become an increasingly important area of research. To date, an ideal material for the interior walls of fusion devices has not yet been found — but the work of Zhili Zhang, associate professor of mechanical, aerospace, and biomedical engineering, may help change that.

"Controlled fusion has some problems. Basically you have to create a very hot gas, so you generate ionized gases called plasmas," said Zhang. "The plasmas will bombard a metal wall and the wall will be etched. The goal is to find a material to hold the plasma, so now the big research problem is the plasma-wall interaction."

Zhang's JDRD project proposes to provide more accurate measurements of plasma-wall interactions in the new ORNL Proto-MPEX, an experimental facility designed to help test materials for their fusion containment capabilities. Zhang's team will contribute to this goal by providing real-time measurement data for the testing materials.

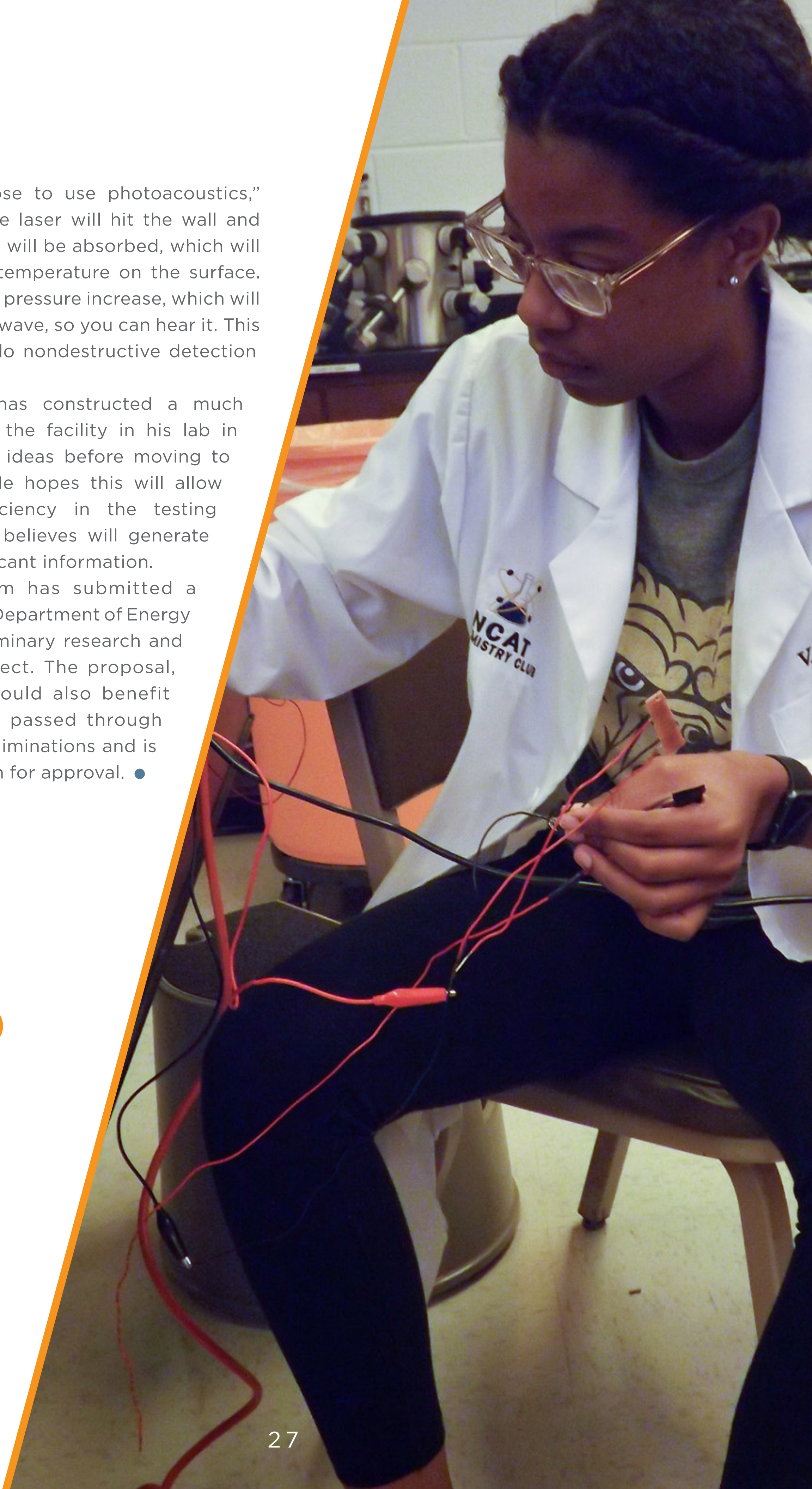
"You know the material will be impacted by the plasma. It's a very fast process. Plasma will etch the wall within almost a millisecond, so how can you provide in situ measurements of the plasma-wall interactions?" said Zhang.

Theodore Biewer, Zhang's partner and a senior research scientist at ORNL, will be investigating this problem by taking surface measurements while his team takes gas phase measurements.

“We also propose to use photoacoustics,” said Zhang. “So the laser will hit the wall and some of the energy will be absorbed, which will increase the local temperature on the surface. That will generate a pressure increase, which will lead to an acoustic wave, so you can hear it. This is a good way to do nondestructive detection on the surface.”

Zhang’s team has constructed a much smaller version of the facility in his lab in order to test their ideas before moving to the Proto-MPEX. He hopes this will allow for improved efficiency in the testing process, which he believes will generate scientifically significant information.

The LDRD team has submitted a proposal to the US Department of Energy based on the preliminary research and design of the project. The proposal, which if funded could also benefit Zhang’s work, has passed through the first round of eliminations and is under consideration for approval. ●



STUDENT SUPPORT

Integral to the charter of the Science Alliance is this principle: Science Alliance funding will be used to "provide incentives to attract and retain the highest quality students and strengthen the educational opportunities for both UT and ORNL."

Consequently, each year a portion of the Science Alliance's funding is distributed directly to two colleges within the university with the express purpose of supporting graduate and undergraduate education and research. 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 projects.

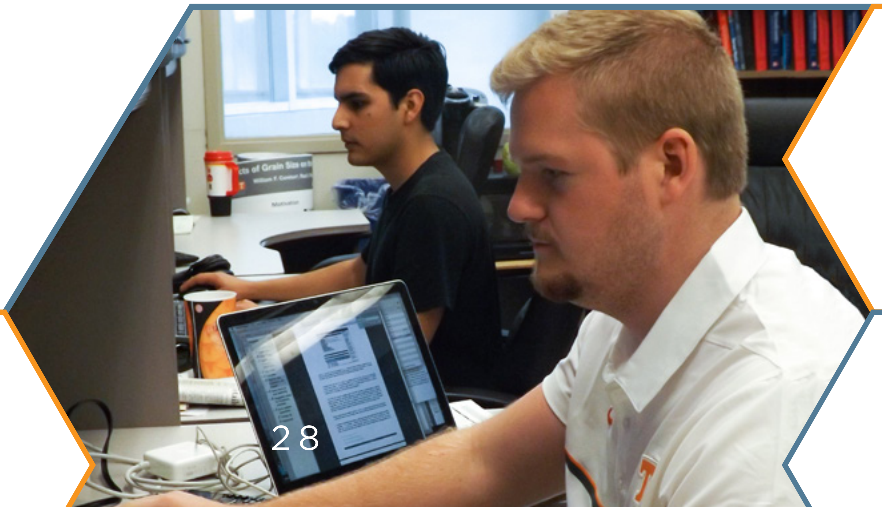
Amanda Haglund, under the direction of Veerle Keppens, has conducted extensive research into the creation of new magnetic materials for transistors. As part of her work, Haglund has gained invaluable experience in the synthesis of these materials as well as ionic liquid testing of 2D materials.

Jeremiah Johnson's graduate student Brittni Kelley has been coordinating the collection of *Campylobacter* strains necessary to conduct Johnson's research. She has worked with the US Food and Drug Administration and the Tennessee Department of Health as well as UT's College of Veterinary Medicine. Additionally, Kelley extracts genomic DNA from the *Campylobacter* strains for sequencing at Indiana University's Center for Genomics and Bioinformatics. Three days a week, she commutes to ORNL for training. Johnson expects she will become proficient in whole-genome analysis by the end of the calendar year.

William Cureton, a graduate student working with Maik Lang, is helping design the modeling system Lang hopes to use as a testing ground for ORNL's ICE-MAN computer platform. In addition to receiving a badge at ORNL, Cureton will assist Oak Ridge scientists in the creation of a user manual for the computer platform.

Christopher Baker's graduate students Larry Warfield and Sara Barker have been responsible for providing the protocol necessary to create the microfluidic chips integral to Baker's sensor design. Both students are receiving hands-on training in the creation of new technologies.

Many students funded by the Science Alliance are actively collaborating with ORNL scientists. They have earned additional funding for their work from a variety of sources, including the US Department of Energy, the National Science Foundation, the National Nuclear Security Administration, and the Army Research Office Young Investigator Program. The contributions made by these scholars to each supported project ensure the University of Tennessee, as well as the state of Tennessee, a substantial foothold in the future of the nation's scientific community. ●



DEPARTMENT	TOTAL SUPPORT	TYPE OF SUPPORT	# OF STUDENTS	HIGHLIGHTS
Biology	300,454	GTA/GRA	33	Nearly two-thirds of supported students are affiliated with ORNL via direct collaboration or UT faculty members, and have worked on a total of 18 publications. One student was awarded the Penley Fellowship Award. Another presented at the American Association for Cancer Research Annual Meeting.
Chemistry	159,964	Graduate Student Trainers/ GTA	7 25	Approximately one-third of students work with mentors with ORNL collaborations. Students are also working on NSF, DOE, NIH and Army sponsored projects. They have authored 24 publications.
Earth & Planetary Sciences	35,653	GTA/GRA	8	Supported students have presented 4 posters and 8 papers at conferences in their field. Half of the students have an affiliation with ORNL and one worked on an experiment at the High Flux Isotope Reactor
Electrical Engineering & Computer Sciences	93,396	GTA/GRA	11	Students are working on DOD and NSF projects and have generated five publications. One student published a how-to for high performance computers using Raspberry Pi.
Geography	10,100	Graduate Student Fellowship	4	100% of funded students have a relationship with ORNL, three of whom have collaborated on a project there. Supported students have produced five publications.
Math	89,000	GTA/GRA	24	Four of the supported students have worked with ORNL, including in the Center for Nanophase Materials Science and the Computer Science and Mathematics Division. Three students have been a part of Distinguished Scientist Clayton Webster's group.
Physics	222,500	GTA	29	The majority of students have a relationship with either ORNL or one of the UT-ORNL Joint Institutes such as the Joint Institute for Advanced Manufacturing. One student received the DOE Office of Science Graduate Student Research Award.
Psychology	10,000	GTA/GRA	2	Both supported students are affiliated with ORNL via a supervising faculty member. They have contributed to four presentations and two publications.

ELBIO DAGOTTO

"Pressure-driven phase transition from antiferromagnetic semiconductor to nonmagnetic metal in two-leg ladders AFe2X3 (A=Ba or K, X=S or Se)." Yang Zhang, Lingfang Lin, Jun-Jie Zhang, **Elbio Dagotto**, and Shuai Dong, *Phys. Rev. B* 95, 115154 (2017).

TAKESHI EGAMI

"Mechanical Deformation in Metallic Liquids and Glasses: From Atomic Bond Breaking to Avalanches", **T. Egami**, Y. Fan and T. Iwashita, in *Avalanches in Functional Materials and Geophysics*, ed. E. Salje, A. Saxena and A. Planes (Springer Verlag, Berlin, 2016) Chapt. 10, pp. 199-225.

"Alex and the Origin of High-Temperature Superconductivity", **T. Egami**, in *High-T_C Copper Oxide Superconductors and Related Novel Materials*, ed. A. Bussmann-Holder et al. Springer Series in Materials Science 255 (Springer Verlag, 2017) Chapter 4, pp. 35-46, ISBN 978-3-319-52675-1.

"Deformation in Metallic Glasses Studied by Synchrotron X-Ray Diffraction", **T. Egami**, Y. Tong and W. Dmowski, *Metals*, 6, 22 (2016).

"Measurements of Structural and Chemical Order in $Zr_{80}Pt_{20}$ and $Zr_{77}Rh_{23}$ Liquids", M. L. Johnson, M. E. Blodgett, K. A. Lokshin, N. A. Mauro, J. Neuefeind, C. Pueblo, D. G. Quirinale, A. J. Vogt, **T. Egami**, A. I. Goldman and K. F. Kelton, *Phys. Rev. B*, 93, 054203 (2016).

"Electrostatic Levitation Facility Optimized for Neutron Diffraction Studies of High Temperature Liquids at a Spallation Neutron Source", N. A. Mauro, A. J. Vogt, K. S. Derendorf, M. L. Johnson, G. Rustan, D. Quirinale, K. Lokshin, J. C. Neuefeind, Ke An, Xun-Li Wang, A.I. Goldman, **T. Egami** and K.F. Kelton, *Rev. Sci. Instrum.* **87**, 013904 (2016).

"Onset of Cooperative Dynamics in an Equilibrium Bulk Metallic Glass-Forming Liquid Revealed by Mean Diffusion Coefficient Measurement", A. Jaiswal, S. O'Keeffe, R. Mills, A. Podlesynak, G. Ehlers, W. Dmowski, K. Lokshin, **T. Egami** and Y. Zhang, *J. Phys. Chem. B* 120, 1142 (2016).

"How to Characterize Disorder", **T. Egami**, *Nucl. Instrum. Method B*, 374, 2 (2016).

"Correlation between Fragility and Arrhenius Crossover Phenomenon in Metallic, Molecular, and Network Liquids", A. Jaiswal, **T. Egami**, K. F. Kelton, K. S. Schweizer and Y. Zhang, *Phys. Rev. Lett.* 117, 205701 (2016).

"Observation of Dynamic Atom-Atom Correlation in Liquid Helium in Real Space", W. Dmowski, S. O. Diallo, K. Lokshin, G. Ehlers, G. Ferré, J. Boronat and **T. Egami**, *Nature Communications*, 8, 15294 (2017); doi: 10.1038/ncomms15294.

"Energy Landscape-Driven Nonequilibrium Evolution of Inherent Structure in Disordered Material", Yue Fan, T. Iwashita, and **T. Egami**, *Nature Communications*, 8, 15417 (2017); doi: 10.1038/ncomms15417.

VEERLE KEPPENS

"Impact of gate geometry on ionic liquid gated ionotronic systems", A. T. Wong, J. H. Noh, P. R. Pudasaini, B. Wolf, N. Balke, A. Herklotz, Y. Sharma, **A. V. Haglund**, S. Dai, D. Mandrus, P. D. Rack, and T. Z. Ward, *APL Materials* 5, 042501 (2017)

"Ionic Liquid Activation of Amorphous Metal-Oxide Semiconductors for Flexible Transparent Electronic Devices", Pushpa Raj Pudasaini, Joo Hyon Noh, Anthony T. Wong, Olga S. Ovchinnikova, **Amanda V. Haglund**, Sheng Dai, Thomas Zac Ward, David Mandrus, Philip D. Rack, *Advanced Functional Materials* 26 (17) 2820-2825 (2016).

JIMMY MAYS

"Unexpected Molecular Weight Effect in Polymer Nanocomposites", Shiwang Cheng, Adam P. Holt, Huiqun Wang, Fei Fan, Vera Bocharova, Martin Halie, Thusitha Etampawala, Benjamin Tyler White, Tomonori Saito, Nam-Goo Kang, Mark D. Dadmun, **Jimmy W. Mays**, and Alexei P. Sokolov, *Phys. Rev. Lett.*, 116, 038302 (2016)

"All-Acrylic Multigraft Copolymers: Effect of Side Chain Molecular Weight and Volume Fraction on Mechanical Behavior", A. Goodwin, W. Wang, N.-G. Kang, Y. Wang, K. Hong, and **J. W. Mays**, *Ind. Eng. Chem. Res.*, 54, 9566 - 9576 (2015).

BLICATIONS

"Fluorinated Bottlebrush Polymers Based on Poly(trifluoroethyl methacrylate): Synthesis and Characterization", Yuewen Xu, Weiyu Wang, Yangyang Wang, Jiahua Zhu, David Uhrig, Xinyi Lu, Jong K. Keum, **Jimmy W. Mays** and Kunlun Hong, *Polymer Chemistry*, *7*, 680 – 688 (2016).

"The Role of Nanoparticle Rigidity on the Diffusion of Linear Polystyrene in a Polymer Nanocomposite", Brad Miller, Adam E. Imel, Wade Holley, Durairaj Baskaran, **J. W. Mays**, and Mark D. Dadmun, *Macromolecules*, 48, 8369 - 8375 (2015).

"Solution Properties of Architecturally Complex Multiarm Star Diblock Copolymers in a Non-selective and Selective Solvent for the Inner Block", J. L. Davis, X. Wang, K. Bornani, J. P. Hinestrosa, **J. W. Mays**, and S. M. Kilbey, II, *Macromolecules*, 49, 2288 – 2297 (2016).

"Failure of Tube Models, and Success of a Slip-Link Model, to Predict the Linear Viscoelasticity of Star/Linear Blends", Priyanka S. Desai, Beom-Goo Kang, Maria Katzarova, Ryan Hall, Qifan Huang, Sanghoon Lee, Taihyun Chang, David C. Venerus, **Jimmy Mays**, Jay D. Schieber, and Ronald G. Larson, *Macromolecules*, 49, 4964 - 4977 (2016).

"Polymerization in Ionic Liquids", H. Zhang, P. K. Behera, N. K. Singha, K. Hong, and **J. W. Mays**, in *Encyclopedia of Polymer Science and Technology*, John Wiley & Sons, 2015.

"High Temperature Thermoplastic Elastomers Synthesized by Living Anionic Polymerization in Hydrocarbon Solvent at Room Temperature", Weiyu Wang, Ralf Schlegel, Benjamin T. White, Katherine Williams, Dimitry Voyloy, Carlos A. Steren, Andrew Goodwin, E. Bryan Coughlin, Samuel Gido, Mario Beiner, Kunlun Hong, Nam-Goo Kang, and **Jimmy Mays**, *Macromolecules*, 49, 2646 - 2655 (2016).

"Effect of Molecular Weight on the Ion Transport Mechanism in Polymerized Ionic Liquids", Fan, Fei; Wang, Weiyu; Holt, Adam; Feng, Hongbo; Uhrig, David; Lu, Xinyi; Hong, Tao; Kang, Nam-Goo; Wang, Yangyang; **Mays, Jimmy W.**; Sokolov, Alexei, *Macromolecules*, 49, 4557 - 4570 (2016).

"Anionic Polymerization of Oxadiazole-Containing 2-Vinylpyridine by Precisely Tuning Nucleophilicity and the Polyelectrolyte Characteristics of the Resulting Polymers", Goodwin, Andrew; Nelson, Kimberly; Wang, Weiyu; Yu, Yong-Guen; Lee, Jae-Suk; Mahurin, Shannon; Dai, Sheng; **Mays, Jimmy W.**; Kang, Nam-Goo, *Macromolecules*, 49, 6213 - 6225 (2016).

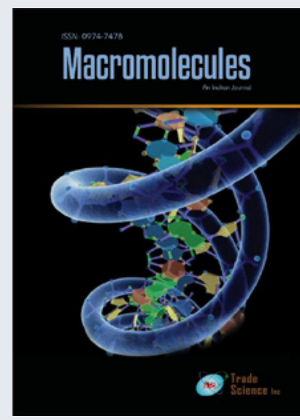
"Effect of Solvent/Polymer Infiltration and Irradiation on Microstructure and Tensile Properties of Carbon Nanotube Yarns", Nitilaksha Hiremath; Xinyi Lu; Maria Cecilia Evora; Amit Naskar; **Jimmy Mays**; Gajanan Bhat, *J. Mater. Sci.*, 51, 10215 - 10228 (2016).

"Recent Developments in Carbon Fibers and Carbon Nanotube-Based Fibers - A Review", Nitilaksha Hiremath, **Jimmy Mays**, and Gajanan Bhat, *Polymer Reviews*, 57, 339 – 368 (2017).

"Impact of Tuning CO_2-philicity in Polydimethylsiloxane-Based Mambranes for Carbon Doixide Separation", Tao Hong, Sabornie Chatterjee, Shannon Mahurin, Fei Fan, Ziqi Tian, De-en Jiang, Brian Long, **Jimmy Mays**, Alexei P. Sokolov, Tomonori Saito, *J. Membr. Sci.*, 530, 213 - 219 (2017).

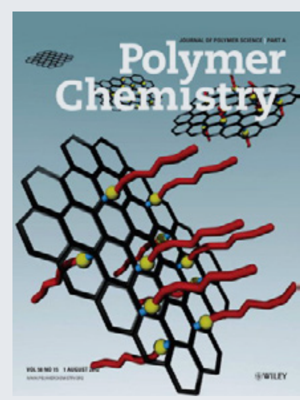
"Tailor-made Thermo-reversible Functional Polymer via RAFT Polymerization in an Ionic Liquid: A Green and Remarkably Fast Polymerization Process", Nikhil K. Singha, Nabendu B. Pramanik, Prasanta K. Behera, Arindam Chakrabarty, **Jimmy W. Mays**, *Green Chemistry*, 18, 6115 - 6122 (2016).

"Poly(adamantyl acrylate): Living Anionic Polymerization, Block Copolymerization, and Thermal Properties", N. Kang, W. Lu, C. Huang, K. Hong, and **J. W. Mays**, *Macromolecules*, 49, 9406 - 9414 (2016).



"2-Isopropenyl-2-Oxazoline: Well-defined Homopolymers and Block Copolymers via Living Anionic Polymerization", H. Feng, M. Changez, K. Hong, **J. W. Mays**, and N. Kang, *Macromolecules*, 50, 54 - 62 (2017).

"Interfacial Properties of Polymer Nanocomposites: Role of Chain Rigidity and Dynamic Heterogeneity Length Scale", Shiwang Cheng, Bobby Carroll, Wei Lu, Fei Fan, Jan-Michael Carrillo, Halie Martin, Adam P. Holt, Vera Bocharova, **Jimmy W. Mays**, Bobby G. Sumpter, Mark Dadmun, and Alexei P. Sokolov, *Macromolecules*, 50, 2397 - 2406 (2017).



"Gas Separation Mechanism of CO_2-Selective Amidoxime- Poly (1-trimethylsilyl-1-propyne) Membranes", Hongbo Feng, Tao Hong, Shannon M. Mahurin, Konstantinos D. Vogiatzis, Kevin Gmernicki, Brian Long, **Jimmy W. Mays**, Alexei P. Sokolov, Nam-Goo Kang, and Tomonori Saito, *Polymer Chemistry*, 8, 3341 - 3350 (2017).

"Improving Mechanical Properties of Carbon Nanotube Fibers through Simultaneous Solid-State Cycloaddition and Crosslinking", N.-G. Kang, X. Lu, N. Hiremath, K. Hong, M. Evora, V. Ransom, A. Naskar, G. Bhat, and **J. Mays**, *Nanotechnology*, 28, 145603 (2017).

"The Tracer Diffusion Coefficient of Soft Nanoparticles in a Linear Polymer Matrix", A. Imel, S. Rostom, D. W. Holley, D. Baskaran, **J. Mays**, and M. Dadmun, *RSC Advances*, 7, 15574 - 15581 (2017).

"Investigations on the Phase Diagram and Interaction Parameter of Poly(styrene-b-1,3-cyclohexadiene) Copolymers", K. Misichronis, J. Chen, A. Imel, R. Kumar, J. Thostenson, K. Hong, M. Dadmun, B. G. Sumpter, J. G. Kennemur, N. Hadjichristidis, **J. W. Mays**, and A. Avgeropoulos, *Macromolecules*, 50, 2354 - 2363 (2017).

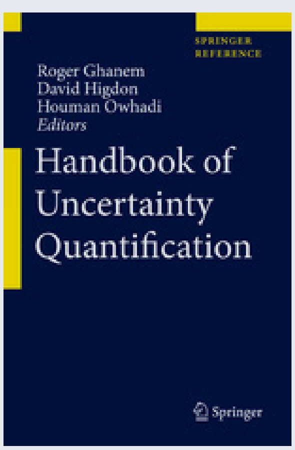
"Thermoplastic Elastomers based on Block, Graft and Star Copolymers", Weiyu Wang, Wei Lu, Nam-Goo Kang, **Jimmy Mays**, and Kunlun Hong, Elastomers, ISBN 978-953-51-5427-3, *Intech Publishers*, 2017.

"Functional Polymers by Reversible Deactivation Radical Polymerisation: Synthesis and Applications", Edited by Nikhil Singha and **Jimmy W. Mays**, *Smithers Rapra Publishers*, ISBN 978-1-91024-255-1, June 30, 2017.

CLAYTON WEBSTER

"Sparse collocation methods for stochastic interpolation and quadrature Max Gunzburger", **C G Webster**, and Guannan Zhang.. In *Handbook of Uncertainty Quantification*, pages 1–46. Springer International Publishing, 2016.

"A sparse grid method for Bayesian uncertainty quantification with application to Large Eddy Simulation turbulence models", H. Tran, **C. G. Webster**, and G. Zhang.. In *Sparse Grids and Applications - Stuttgart 2014*, volume 109 of *Lecture Notes in Computational Science and Engineering*, pages 291–313. Springer International Publishing, 2016.



"An efficient meshfreee implicit filter for nonlinear filtering problems", F. Bao, Y. Cao, **C. G. Webster**, and G. Zhang. *International Journal for Uncertainty Quantification*, 6:19–33, 2016.

"Fast and efficient stochastic optimization for analytic continuation", [25] F. Bao, Y. Tang, M. Summers, G. Zhang, **C. G. Webster**, V. Scarola, and T. A. Maier. *Physical Review B*, 94(12):125–149, 2016.

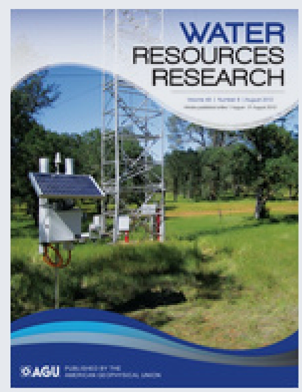
"Polynomial approximation via compressed sensing of high-dimensional functions on lower sets", A. Chkifa, N. Dexter, H. Tran, and **C. G. Webster**. *Mathematics of Computation*, 2016. To appear (arXiv:1602.05823).

"Explicit cost bounds of stochastic Galerkin approximations for parameterized PDEs with random coefficients", N. C. Dexter, **C. G. Webster**, and G. Zhang. *Computers & Mathematics with Applications*, 71(11):2231–2256, 2016.

"Accelerating stochastic collocation methods for partial differential equations with random input data", D. Galindo, P. Jantsch, **C. G. Webster**, and G. Zhang. *SIAM/ASA Journal on Uncertainty Quantification*, 4(1):1111–1137, 2016.

"On the Lebesgue constant of weighted Leja points for Lagrange interpolation on unbounded domains", P. Jantsch, **C. G. Webster**, and G. Zhang. *Constructive Approximation*, 2016. Submitted (arXiv:1606.07093).

"An improved multilevel monte carlo method for estimating probability distribution functions in stochastic oil reservoir simulations", D. Lu, G. Zhang, **C. G. Webster**, and C. Barbier. *Water Resources Research*, 52(12):9642–9660, 2016.



"A dynamically adaptive sparse grid method for quasi-optimal interpolation of multidimensional functions", M. K. Stoyanov and **C. G. Webster**. *Computers & Mathematics with Applications*, 71(11):2449–2465, 2016.

"Hyperspherical sparse approximation techniques for high-dimensional discontinuity detection", G. Zhang, **C. G. Webster**, M. Gunzburger, and J. Burkardt. *SIAM Review*, 58(3):517–551, 2016.

"Numerical methods for a class of nonlocal diffusion problems with the use of backward SDEs", G. Zhang, W. Zhao, **C. G. Webster**, and M. Gunzburger. *Computers & Mathematics with Applications*, 71(11):2479–2496, 2016.

"Reduced basis methods for nonlocal diffusion problems with random input data", Q. Guan, M. Gunzburger, **C. G. Webster**, and G. Zhang. *Computer Methods in Applied Mechanics and Engineering*, 317:746–770, 2017.

“Analysis of quasi-optimal polynomial approximations for parameterized PDEs with deterministic and stochastic coefficients”, H. Tran, **C. G. Webster**, and G. Zhang. *Numerische Mathematik*, 45(4):1–43, 2017.

BOB HATCHER

“Confirmation of the southwest continuation of the cat square terrane, southern appalachian inner piedmont, with implications for middle paleozoic collisional orogenesis.”Huebner, M. T., **Hatcher, R. D.**, & Merschat, A. J. (2017). *American Journal of Science*, 317(2), 95-176. doi:10.2475/02.2017.01

“Geologic and kinematic insights from far-traveled horses in the Brevard fault zone, southern Appalachians: in Law, R. D., Stowell, H. T., Thigpen, J. R., eds.” **Hatcher, R. D.**, Huebner, M. T., Rehrer, J. R., Acker, L. L., Fullagar, P. D., Liu, A., & Goad, P. L. (2017). *Linkages and Feedbacks in Orogenic Processes* based on the 2014 Penrose Conference.

“The Paleozoic tectonic evolution of the western Blue Ridge, southern Appalachians: A critical examination of longstanding conflicts in a polydeformed system in Law, R. D., Stowell, H. T., Thigpen, J. R., eds.” **Hatcher, R. D.** (2017). *Linkages and Feedbacks in Orogenic Processes* based on the 2014 Penrose Conference.

“Transition from B- to A-subduction during closing of the Rheic remnant ocean: New geochronologic and geochemical data marking Acadian/Neoacadian orogenesis and accretion of the Carolina superterrane, southern Appalachians, in Law, R. D., Stowell, H. T., Thigpen, J. R., in Law, R. D., Stowell, H. T., Thigpen, J. R., eds.” **Hatcher, R. D.**, & Huebner, M. T. (2017). *Linkages and Feedbacks in Orogenic Processes* based on the 2014 Penrose Conference.

“Temporal and spatial distribution of Paleozoic metamorphism in the southern Appalachian Blue Ridge and Inner Piedmont delimited by ion microprobe U-Pb ages of metamorphic zircon, in Law, R. D., Stowell, H. T., Thigpen, J. R., eds.” **Hatcher, R. D.**, Merschat, A. J., Bream, B. R., Huebner, M. T., & Miller, C. F. (2017). *Linkages and Feedbacks in Orogenic Processes* based on the 2014 Penrose Conference.

“Reevaluating the age of the Walden Creek Group and the kinematic evolution of the western blue ridge, Southern Appalachians.” Thigpen, J. R., **Hatcher, R. D.**, Kah, L. C., & Repetski, J. E. (2016). *American Journal of Science*, 316(3), 279-308. doi:10.2475/03.2016.03

“Paleoseismic evidence for multiple Mw ≥ 6 earthquakes in the East Tennessee seismic zone during the late Quaternary.” **Hatcher, R. D.**, Warrell, K. F., Cox, R. T., Vaughn, J. D., & Counts, R. (n.d.). *Bulletin of the Seismological Society of America*.

Structural Geology: Principles, Concepts and Problems (3rd ed.). **Hatcher, R. D.**, & Bailey, C. M. (2018). Oxford University Press.

“Geologic and kinematic insights from far-traveled horses in the Brevard fault zone, southern Appalachiansi n Law, R.D., Stowell, H. T., and Thigpen, J. R., eds.,” **Hatcher, R. D.**, Huebner, M. T., ., Rehrer, J. R., Acker, L.L., Fullagar, P. D., Liu, A.., & Goad, P. L. (2017). *Linkages and Feedbacks in Orogenic Processes*. Geological Society of America.

“The Paleozoic tectonic evolution of the western Blue Ridge, southern Appalachians: A critical examination of longstanding conflicts in a polydeformed system in Law, R.D., Stowell, H. T., and Thigpen, J. R., eds.,” Thigpen, J. R.., & **Hatcher, R. D.** (2017). *Linkages and Feedbacks in Orogenic Processes*. Geological Society of America.

“Transition from B- to A-subduction during closing of the Rheic remnant ocean: New geochronologic and geochemical data marking Acadian/Neoacadian orogenesis and accretion of the Carolina superterrane, southern Appalachians, in Law, R. D., Stowell, H. T., and Thigpen, J. R., eds.,” Huebner, M. T.., & **Hatcher, R. D.** (2017). *Linkages and Feedbacks in Orogenic Processes*. Geological Society of America.

“Temporal and spatial distribution of Paleozoic metamorphism in the southern Appalachian Blue Ridge and Inner Piedmont delimited by ion microprobe U-Pb ages of metamorphic zircon, in Law, R. D., Stowell, H. T., and Thigpen, J. R., eds.,” Merschat, A. J.., Bream, B. R., Huebner, M. T.., **Hatcher, R. D.**, & Miller, C. F.. (2017). *Linkages and Feedbacks in Orogenic Processes*. Geological Society of America.

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