THE UNIVERSITY OF TENNESSEE KNOXVILLE

SCIENCE ALLIANCE

UT - ORNL Science Alliance Annual Report

July 1, 2014 - June 30, 2015

UT - ORNL Science Alliance

July 1, 2014 - June 20, 2015

Annual Report

CONTENTS

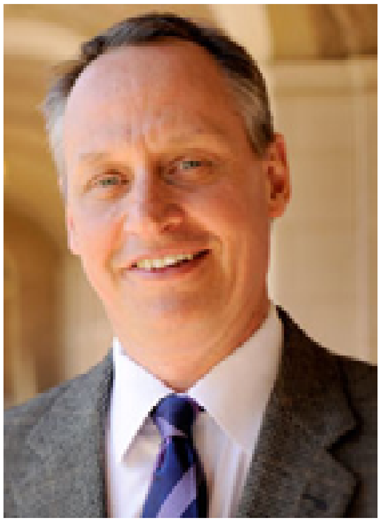
Vice Chancellor for Research & Engagement
Taylor Eighmy

Associate Vice Chancellor for Research Development
Janet Nelson

Assistant Vice Chancellor	Elizabeth Neilson
Business Manager	Betty Carmon
Administrative Specialist	Jennifer Brown

This report to the Tennessee Higher Education Commission is a publication of the Science Alliance, a Center of Excellence at the University of Tennessee, Knoxville.

Vice Chancellor for Research & Engagement



The Science Alliance is absolutely critical to the future of the University of Tennessee, Knoxville and Oak Ridge National Laboratory (ORNL). UT, along with Battelle Memorial Institute, jointly operates ORNL, the largest DOE Office of Science national lab. More importantly, UT and ORNL have a long history of collaboration dating back to 1946. Since that time, significant progress has been made in our collaborative research and development relationship: we presently have five joint institutes, 214 joint faculty, a robust Bredesen Center interdisciplinary Ph.D. graduate program with over 120 students enrolled in the energy science and engineering disciplines.

Moreover, ORNL scientists and UT Knoxville faculty are collaborating on large initiatives in advanced manufacturing, materials science, high performance computing, bioenergy science, and neuroscience to name a few. A common feature to many of our recent collaborations includes evolving partnerships with Eastman Chemical Company, Volkswagen, Boeing, Ford, Dow, DowAksa, FedEx, the Kavli Foundation, and the Bill and Melinda Gates Foundations.

Looking ahead to 2020, a new contract is expected to be awarded by U.S. Department of Energy to operate ORNL. UT and Battelle Memorial Institute are the incumbent contractors (operating under the UT-Battelle LLC) and it is critical for UT and ORNL to maximize our opportunities to further grow and add value to our collaboration. Significant state investments assisted this LLC when the contract was awarded in 2000. Given this, it is worth elaborating - using just three examples - on how the Science Alliance funding is also critical to both our relationship and to this continued investment in our collaborations.

Our Distinguished Scientists - Drs. Dagotto, Egami, Hatcher, Joy, and Mays - brought a total of $6.7 million in new research awards to UT in fiscal year 2015 with $1.1 million in matching funds from ORNL. Each of these faculty are playing prominent roles in discovery science, scholarship, graduate education, and professional recognition.

In January 2015, President Obama came to Clinton, Tennessee to announce the Nation's fifth Institute for Manufacturing Innovation focused on composites. As part of the larger National Network of Manufacturing Innovation, this 123-member, six state effort joins those around 3-D printing, digital manufacturing, lightweight metals, and wide band gap electronics. The Institute for Advanced Composites Manufacturing Innovation (IACMI) was launched at a conference in June 2015 with over 400 attendees. Science Alliance funds are being used as cost share to leverage federal and private sector investment at almost 3:1 to help UT.

In July 2015, Eastman announced that UT had joined Eastman's Innovation Network (EIN); one of three U.S. universities to belong to EIN. Critical to the research and development planned under the EIN will be the neutron science user facilities (the Spallation Neutron Source or SNS and the High Flux Isotope Reactor or HFIR) at ORNL. The relationship with Eastman is occurring through the UT-ORNL Joint Institute for Neutron Sciences. Eastman is funding UT through a master research agreement for $0.8M.

We expect to continue to leverage Science Alliance support in cost sharing on large federal awards, in closely aligned research and development investment from UT and ORNL, and in industrial support for research and technology transfer. The future between UT and ORNL is bright and the Science Alliance funding is critical to our continued growth and success.

Taylor Eighmy

Overview

The Science Alliance is a Tennessee Center of Excellence established in 1984, and is 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 UT and ORNL together to support technology transfer
- Build areas of common strength
- Provide incentives to attract and retain the highest quality faculty and students
- Strengthen the 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. Science Alliance funds support a variety of critical investments in people and in collaborations.

Much of our current collaborative research emphasizes strategic areas of importance to both organizations. Advanced manufacturing, advanced materials and materials science, neutron science, computational science, big data and data science, and bioinformatics are currently among the most prominent UT-ORNL collaborative areas receiving support. UT-Battelle management of ORNL is also synergistic with this form of investment: many of the investments made with UT-Battelle fees support the joint institutes. Collectively, these are substantial and shared obligations.

The current Science Alliance program reflects investments in both people and research collaboration. Funds are used to support our Distinguished Scientist Program – a precursor to our Tennessee Governor's Chair Program and the cornerstone of Science Alliance programming. They are also used to encourage joint directed research and development (JDRD) between university faculty and students and ORNL scientists. These collaborations join with ORNL's efforts to invest in research through their laboratory-directed research and development (LDRD) funding and Seed funding programs. Science Alliance funds are also used to support graduate student education in sciences and engineering at UT.

Last year the Science Alliance added the Collaborative Cohort Program, a fellowship designed to support collaboration between underrepresented UT junior faculty and ORNL junior scientists. The cohorts work closely with ORNL's newly established Liane B. Russell Fellows and are mentored by faculty and senior scientists, the UT Office of Research and Engagement, ORNL, and DOE participants so as to further advance their research careers.

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 to innovative and groundbreaking collaborations between people. Great science and discovery comes when people–to-people interactions are optimized, not unlike a chemical reaction. A reaction progresses because of collisions and these funds support such interactions. They serve a critical role in leveraging the federal investments made at ORNL and UT in our areas of collaborative research and development.

The bridge to John D. Tickle Engineering building looks out on Ferris and Perkins Halls.

Distinguished Scientist Program

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

Distinguished Scientists hold a tenured professorship at the University of Tennessee; most also hold a Distinguished Scientist appointment at ORNL, nominally half-time at each institution. The appointments include an ongoing discretionary research fund equal to twelve months' salary.

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

Elbio Dagotto

UT Department of Physics and Astronomy
ORNL Division of Materials Science and Technology

Nanoscale dimensions and correlated electronic behavior

Elbio Dagotto primarily uses computational techniques to study transition metal oxides, oxide interfaces, and the recently discovered iron based, high-temperature superconductors. These materials and others studied by his group show promise both for technological applications and for advancing 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 DOE Field Work Proposal, FWP, at ORNL, entitled “Theoretical studies of Complex Collective Phenomena,” which secured a grant from the Department of Energy that supplied $1,992,000 for 18 months to ORNL.

Takeshi Egami

UT Department of Materials Science and Engineering
UT Department of Physics and Astronomy
ORNL Division of Materials Science and Technology

Atomic-scale dynamics of liquids and gases; high temperature superconductivity

The physics of liquids is much less developed than the physics of solids. Takeshi Egami explores new science of liquids and gases using computer simulation (including quantum mechanical calculations) and neutron and synchrotron x-ray scattering experiments.

Egami is currently participating in a number of active collaborations with ORNL scientists, including Department of Energy projects whose fiscal year budgets total more than $2.7 million.

Additionally, Egami has served as Editor for *Advances in Physics* from 2011 to the present and Divisional Associate Editor in Condensed Matter Physics for *Physical Review Letters*.

Robert Hatcher

UT Department of Earth and Planetary Sciences

Structural geology and tectonics of continental crust

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, and conducts related studies to try to answer the question of why there are earthquakes in the eastern U.S.

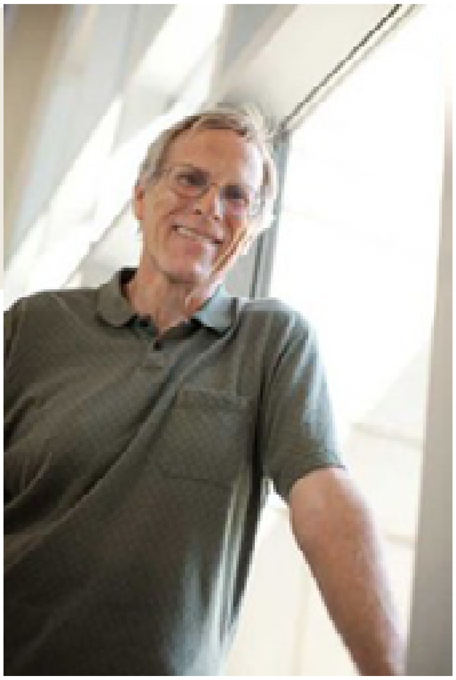
Hatcher is currently serving as Principal Investigator on a Nuclear Regulatory Commission supported project studying Paleoseismology of the East Tennessee Seismic Zone. His collaborations with scientists at the University of Memphis and the U.S. Geological Survey have yielded important information about seismic hazards in East Tennessee.

In 2014 he was the recipient of the Marcus Milling Legendary Geoscientist medal. Additionally, he and scientists from six countries were recognized at the Geological Society of America Penrose Conference.

David Joy

UT Department of Biochemistry and Cellular and Molecular Biology
UT Department of Materials Science and Engineering
ORNL Division of Materials Science and Technology

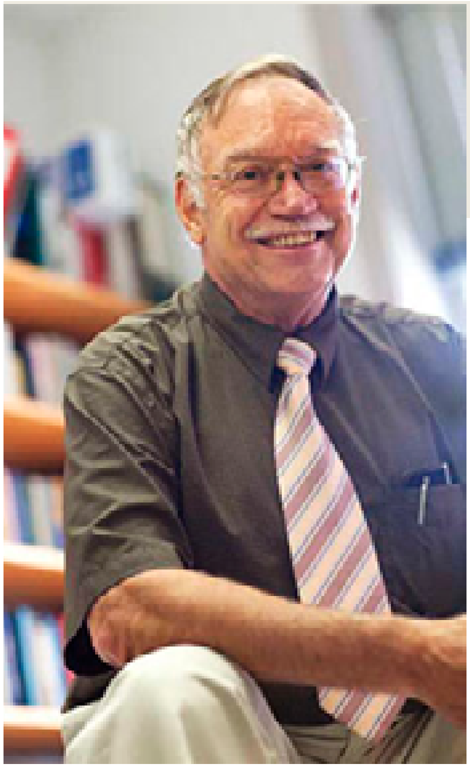
Accurate microscopic and nanoscale imaging



David Joy's research helps create accurate microscopic and nanoscale imaging techniques, including the new, superior performing 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 consistenly 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 dollars 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*.



Joseph Macek

UT Department of Physics and Astronomy
ORNL Physics Division

Electron vortices in simple atomic systems

The probabilites of finding electrons at given points in space are described mathematically in quantum mechanics. Joseph Macek relies on this theory to study what happens to simple fragmented atomic systems when atoms collide.

Macek joined the Science Alliance as a Distinguished Scientist in 1988 when he arrived at UT, and remained a member until his retirement in August of 2014.

Macek's final project under the Science Alliance resulted in multiple publications with several high profile journals, including *Physical Review Letters* and *Few-Body Systems*.

Jimmy Mays

UT Department of Chemistry
ORNL Division of Chemical Sciences

Synthesizing new polymer membranes for fuel cells

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. Additionally, 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, China.

In Memory

Georges Andre Guiochon

September 6, 1931 - October 21, 2014

Internationally renowned scientist in the field of chromatography

Professor in the Department of Chemistry

UT-ORNL Distinguished Scientist 1987 - 2014

External Research Funds Awarded to UT-ORNL Distinguished Scientists in FY15

The following table lists the research funding brought in to The University of Tennessee from external sources by Distinguished Scientists designated as principal investigators on the projects. Distinguished Scientists are also part of investigative teams on many other funded research proposals as well, including research grants awarded to Oak Ridge National Laboratory.

Principal Investigator	Project Name	Project Title	Start Date	End Date	Award Amount	FY15 Expenditures
Dagotto	NSF-DMR-1104386	Computational Studies of Model Hamiltonians for Pnictides and Multiferroic Manganites	09/01/2011	08/31/2014	$420,000	$(3,666)
Dagotto	NSF-DMR-1404375	Hamiltonians for Iron-Based Superconductors in Quasi One-Dimensional Geometrics	09/01/2014	08/31/2017	435,000	72,862
Egami	UT-B 4000126542 Egamii	Dynamics of Biologically Relevant Model Membrane Systems	09/20/2013	08/31/2015	87,210	61,852
Egami	UT-B 4000137944 Egami	Development of Dynamic PDF Method	04/01/2015	09/30/2015	120,000	14,202
Egami	DOE-DE-FG02-08ER46528	Neutron Scattering Research Network for Epscor States - Dept Matching	09/01/2008	09/30/2018	787,696	(105,733)
Egami	DOE-FG02-08ER46528	Neutron Scattering Research Network for Epscor States	9/1/2008	9/30/2015	69,070	5,273
Egami	JINS Enrichment Fund	JINS Enrichment Fund	07/01/2005	12/31/2047	29,000	511
Egami	DOE-DE-FG02-8ER46528-004	Neutron Scattering Research Network for EPSCOR States	09/01/2008	09/30/2015	1,206,550	319,298

External Funding FY15

Principal Investigator	Project Name	Project Title	Start Date	End Date	Award Amount	FY15 Expenditures
Egami	UT-B 4000119538	Physics of Metallic Glasses	01/01/2013	12/31/2015	563,543	163,508
Egami	UT-B 4000131427 Egami	Local Structure by Neutron Diffraction	07/01/2014	06/30/2016	180,000	107,010
Egami	UT-B 4000135651	Neutron Scattering Study of Localized Atomic Vibrations	11/13/2014	10/19/2015	24,994	21,007
Guichon	NSF CHE-1108681	Fundamental Studies in Nonlinear Chromatography	09/19/2011	12/31/2014	350,000	12,141
Hatcher	NRC-HQ-11-G-04-0085 Hatcher	Two-Year Collaborative Research Project to Assess Large Earthquake Seimology in the ETSZ	09/26/2011	09/01/2016	454,706	69,781
Hatcher	USGS G13AC00089 Hatcher	Detailed Geologic Mapping of Quaternary French Broad River Terraces, Eastern Tennessee	05/01/2013	07/31/2014	8,217	1,471
Hatcher	USDI-NS P14AC00244 - Hatcher	Geologic Mapping of the Lancing, Hebbertsburg, and Fo Creek 7.5 minute quadrangle, Wild and Scenic River	04/01/2014	08/31/2015	43,537	29,093
Hatcher	USDI-NPS P15AS00223 - Hatcher	New Geological Map of Chickamauga and Chattanooga National Military Park	08/31/2015	10/31/2016	43,000	-

External Funding FY15

Principal Investigator	Project Name	Project Title	Start Date	End Date	Award Amount	FY15 Expenditures
Joy	SRC-2011-OJ-2122 Joy	Focused Helium Ion Beam Induced Synthesis for Repair, Metrology Sample Preparation, and Lithography	01/01/2011	06/30/2014	111,974	(4,353)
Macek	DOE-DE-FG02-02ER15283-Macek 12 49%	Theory of Atomic Collisions and Dynamics	03/01/2012	2/28/2015	376,000	90,034
Mays	Dow Chemical Co - Jimmy Mays	Unrestricted Research Support	10/30/2002	12/31/2047	35,000	-
Mays	NSF-IIP-1237787	PFI-BIC: Superelastomers Based on Multigraft Copolymers	09/01/2012	08/31/2015	493,258	172,068
Mays	Vanderbilt Univ Sub No. 2016-015735	Improved Carbon Nanotube Fibers through Crosslinking and Densification	01/01/2013	12/31/2015	247,500	108,445
Mays	Vanderbilt Univ Sub No. 2016-015735	Vanderbilt Univ Sub No. 2016-015735	01/01/2013	12/31/2014	154,402	73,494
Mays	Bill & Melinda Gates Fnd OPP1098281 Mays	Ultra-Sensory Condoms Based on New Superelastomer Technology	01/01/2013	10/31/2015	100,000	36,582
Mays	Dow Chemical Co. Synthesis Polyethyl Mays	Sythesis of H Polyethyenes	02/01/2014	12/31/2014	19,228	947
Mays	UT-B 4000136406	Synthesis of Miktoarm Terpolymers	12/29/2014	11/23/2015	70,000	40,092

External Funding FY15

Principal Investigator	Project Name	Project Title	Start Date	End Date	Award Amount	FY15 Expenditures
Mays	UT-B 4000138903	Synthesis of Block Copolymers for Anion Conducting Membranes	05/04/2015	09/30/2015	39,052	14,688
Mays	NSF-EPS-1004083 Mays Yrs 2-5	TN Solar Conversion and Storage Using Outreach, Research and Education (TN-SCORE)	09/06/2011	07/31/2015	204,260	115,480
		Total External Funds			**$6,673,200**	**$1,416,088**
		Total Matching Funds ORNL			**$1,107,112**	**$1,168,604**

Elbio Dagotto
Department of Physics and Astronomy

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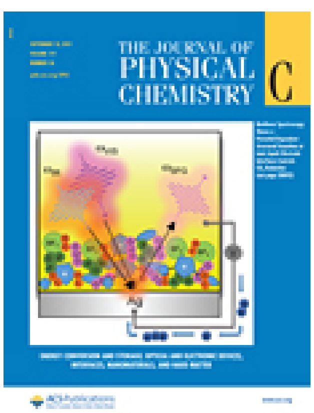

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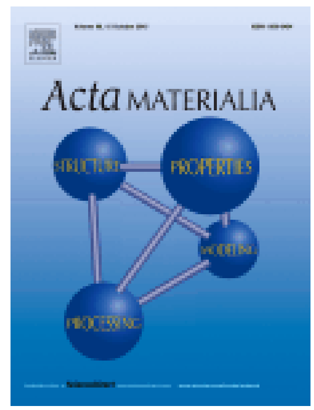

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Robert Hatcher, Jr.

Department of Earth and Planetary Sciences

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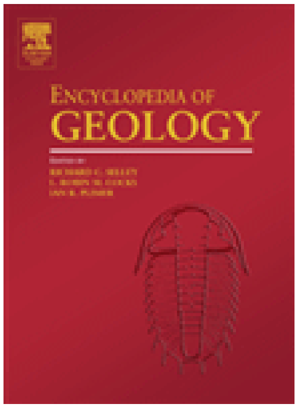

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Jimmy Mays

Department of Chemistry

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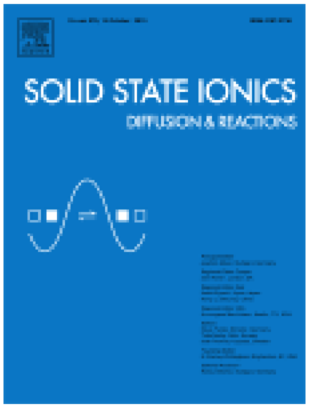

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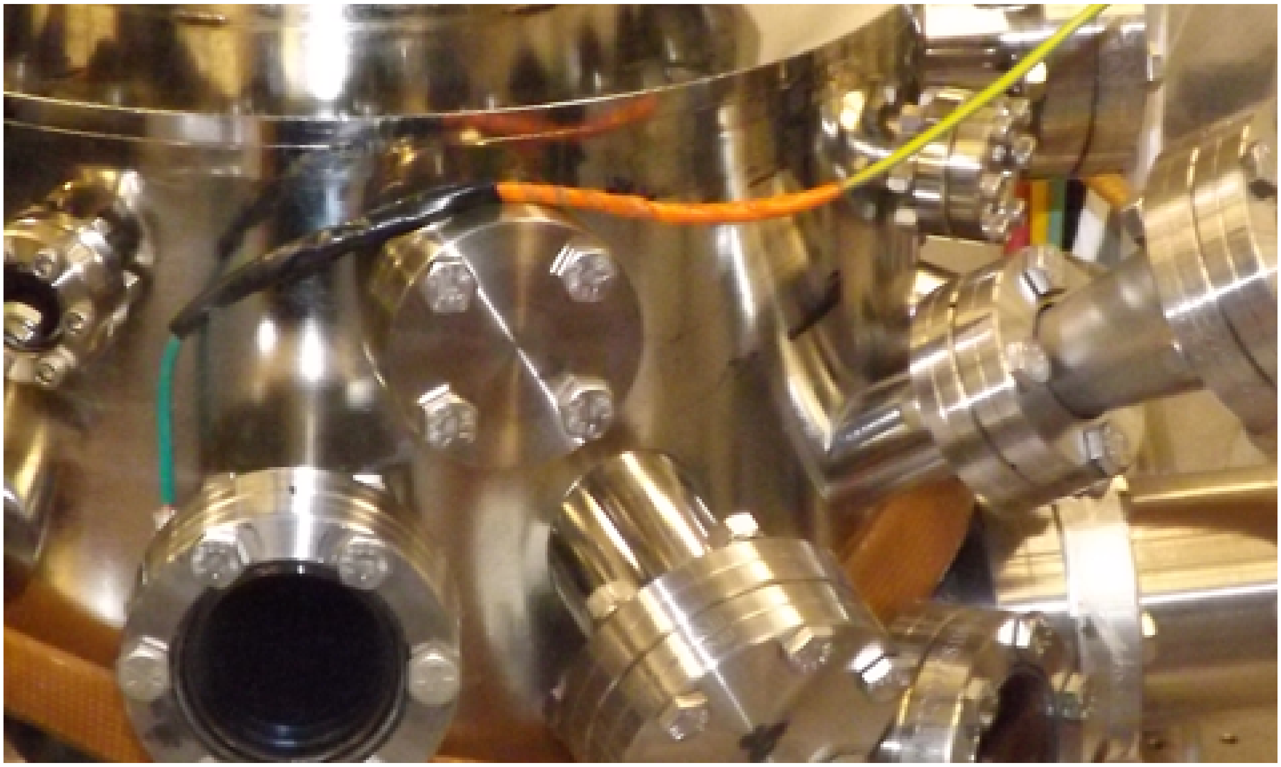
The Science and Engineering Research Facility is a 230,000 square foot facility dedicated to research laboratories utilized by UT scientists across a range of disciplines, including many working on Science Alliance funded projects.

Joint Directed Research and Development



The Joint Directed Research and Development (JDRD) program offers an opportunity for collaborative research with Oak Ridge National Laboratory (ORNL).

A dual UT and ORNL venture, JDRD complements the Laboratory Directed Research and Development program (LDRD) and ORNL Seed Money Fund. The LDRD is a 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 program provides a source of funding for innovative ideas that have the potential to enhance the Laboratory's core scientific and technical competencies, as well as 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 an ORNL component.

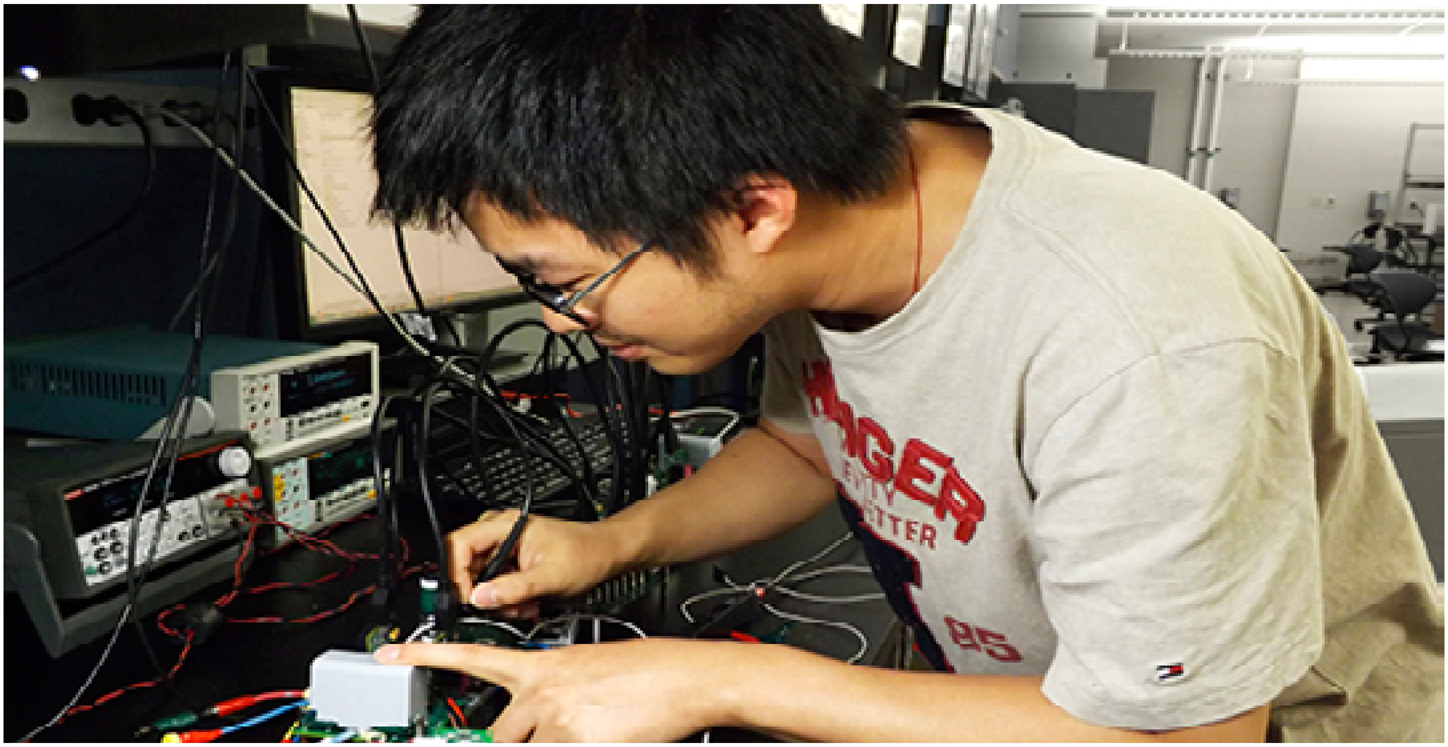
JDRD awards run for two calendar years with a progress assessment at the end of year one to determine if second year funding will be awarded. Second year funding is based on the development of the partnership and the research progress thus far. In CY 2015 the Science Alliance funded nine first year JDRD projects and three second year projects.

Note: JDRD projects operate on a calendar year cycle, while Science Alliance funding is designated on a fiscal year calendar. The following projects were funded in fiscal year 15, which included calendar year 2014 and 2015.

Daniel Costinett

Science Alliance JDRD - ORNL LDRD 1/1/2014-4/30/2016

Targeted drive train DC-DC design for electric vehicles using additive manufacturing and wide band gap semiconductors



Electric vehicles (EVs) have become fixtures in the car market, both in the United States and abroad, but there are hurdles to mass consumer adoption. In addition to continuing to be cost prohibitive to many, EV technology is still in need of advancements in efficiency, particularly at performance levels typical of normal use.

As of December 2014, the U.S. possesses the largest fleet of plug-in electric vehicles in the world, with 291,332 highway capable plug-in electric cars sold since the launch of the Tesla Roadster in 2008. In 2013, the U.S. Department of Energy, launched the "EV Everywhere Grand Challenge," a program designed to spur advancement in electric vehicle technology.

Dr. Daniel Costinett's JDRD team has taken up this challenge with a project that seeks to improve the performance of EVs at standard use levels by working on a new DC-DC drive train system through the design of a new power converter. Costinett's team is taking elements of two currently existing power converters and merging them into a single new system, a design that will be cheaper, smaller and more efficient.

"Right now, everything is built to the worst case scenario," says Costinett. "They're efficient at full power and full speed, but when you get back to more typical use, the efficiency decreases."

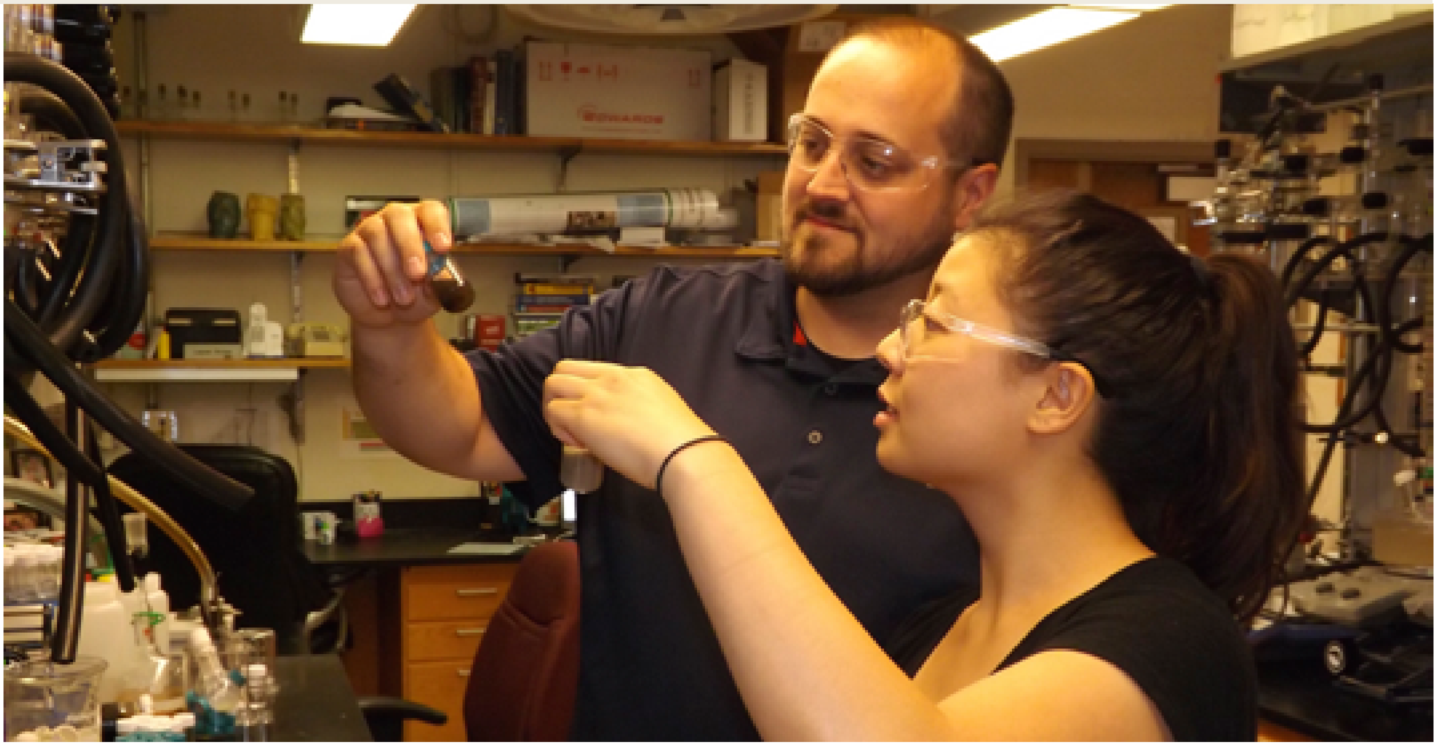
The converter is being designed with an eye toward creating better results for typical use, while maintaining effective functionality at maximum use. Costinett's new configuration should also allow the system to continue operating in the event of converter failure. The team's goal is to create a converter which is both 25% smaller and 40% lower in cost than the current state-of-the-art technology, while reducing total energy losses by 30%.

Costinett's JDRD team is currently working with new materials for transistors, traditionally made with silicon, and has created a scaled down converter prototype for testing, which is yielding promising results. The advances generated by this project could potentially lead to a breakthrough in the electric vehicle cost-performance ratio and facilitate future collaborations between UT and ORNL teams.

Brian Long

Science Alliance JDRD - ORNL LDRD 1/1/2014-12/31/2015

Synthesis and evaluation of advanced poylmeric membranes for carbon dioxide separation



CO_2, or carbon dioxide, is the most prevalent greenhouse gas emission caused by human beings. According to the U.S. Environmental Protection Agency (EPA) in 2011, approximately 6.7 billion metric tons of carbon dioxide was released into Earth's atmosphere as a result of fossil fuel combustion for electricity generation, transportation and other human activities. As a result, the EPA has called for a 30% reduction in greenhouse gas emissions from existing power plants by 2030, which is referred to as the Clean Power Plan.

According to Dr. Brian Long, one of the most effective methods for reducing carbon dioxide emissions for existing power plants is CO_2 capture, or "scrubbing." Unfortunately, these capture mechanisms are currently very energy intensive, creating a vicious cycle of burning electricity to remove the carbon dioxide byproduct of creating electricity. Long's JDRD project could potentially change all of that.

"We are trying to develop low cost plastic membranes that allow the separation of greenhouse gases from other non-harmful gases," said Long. His JDRD team is in the process of designing advanced bilayer membranes that do just that. In its first year, Long's JDRD team made significant advances in membrane mediated CO_2 separation by developing new materials for use in these membrane systems, which function with remarkable efficiency.

"Once the membranes are made, there's almost zero energy input," said Long. The membranes passively filter the gases with no additional power requirements, effectively breaking the energy cycle.

Analysis of these new membranes indicates functionality that can approach, and often exceed Robeson's upper bound, the metric by which all CO_2-separation membranes are evaluated. In the second year of this project, Long's team has manufactured some of the new membranes and begun testing them with new instrumentation that was custom constructed within their labs.

Long's JDRD project has benefited from the work of four graduate students; Kevin Gmernicki, Eunice Hong, Nolan Mitchell and Lauren Brown. Each student has been responsible for meaningful contributions to the project, with Gmernicki and Hong listed as the two primary researchers, each with two publications in progress as a result of this JDRD project.

Haixuan Xu

Science Alliance JDRD - ORNL LDRD 1/1/2014-12/31/2015

Transport properties of interfacial defects in materials

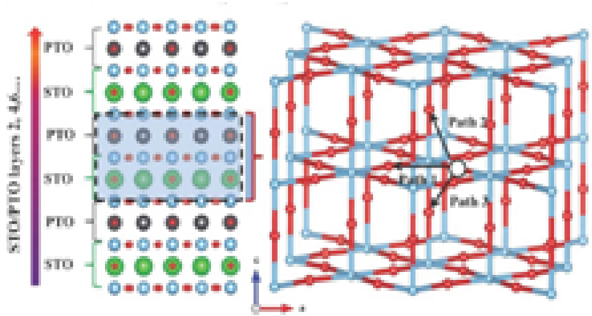
Significant advancements in any field are built on a strong foundational understanding of that field, amassed from years of tireless work. Haixuan Xu's JDRD project is adding to that foundation in the study of materials science.

In an effort to encourage the very type of work undertaken by Xu's team, the Federal government introduced the Materials Genome Initiative, a multi-agency undertaking designed to enable the effort to discover, manufacture and deploy advanced materials at a faster pace and a lower price.

Xu's project uses predictive modeling, logging time on high performance supercomputers to analyze a variety of materials. This is a relatively uncommon practice, as most analyses are conducted with one material at a time, a practice established in the 1980's.

Specifically, his team is investigating novel combinations of oxide materials for creating interfaces with unprecedented properties and functionalities, focusing on the stability and electronic properties of point defects at the interfaces between complex ternary oxides.

Point defects are irregularities found within a lattice structure. These defects don't carry the weight of a negative connotation, but rather they present an opportunity for study. According to Xu, the presence of point defects significantly affects the unusual properties displayed by the oxides, and lacking a fundamental understanding of the effect of point defect dynamics limits the ability to generate particular properties within the interfaces.



The applications for the materials discovered during the course of this necessary foundational research is applicable to a variety of areas, including battery performance, ballistic protection, and new forms of electronics.

Currently in its second year, Xu's project has already yielded one significant publication with several more in progress. Ultimately, Xu hopes his work positions UT for many future research endeavors with the Materials Genome Initiative and other sponsored programs.

Steven M. Abel

Assistant Professor, Department of Chemical and Biomolecular Engineering
Science Alliance JDRD - ORNL Seed 1/1/2015-12/31/2015

Membrane domain formation on nanostructured scaffolds: theory and computational modeling

Computational modeling is an invaluable tool allowing for the study of the behavior of a complex system via computer simulation, providing scientists with an opportunity for accelerated discovery.

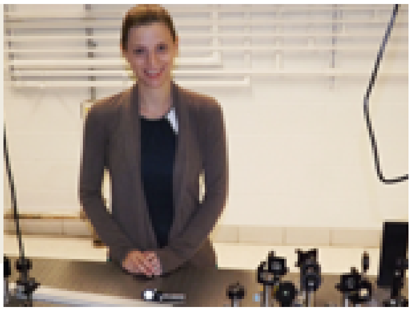
Applying this tool to the study of cellular membranes, Dr. Steven Abel's JDRD team seeks to uncover a deeper fundamental understanding of cell membranes and how they are spatially organized. The cell membrane is the part of a cell that controls its interactions with its environment; what material goes in and out, what proteins at the membrane transmit information about the environment and so forth.

A better understanding of membrane organization could impact a variety of disciplines, ranging from immunology to drug design to the construction of biomimetic materials.

In conjunction with an ORNL team using nanostructured scaffolds to alter lipid bilayers, Abel's team developed mathematical models of the interactions between these scaffolds and cell membranes to determine how the scaffolding's presence affects the lipids.

The computational model created by this project has the potential to benefit future experiments by testing the relative importance of various physical properties and probing parameter space for interesting behavior to guide experimental design.

Tessa R. Calhoun



Assistant Professor, Department of Chemistry
Science Alliance JDRD - ORNL LDRD 1/1/2015-12/31/2015

Imaging nanomaterial interfaces using evanescent wave electronic sum frequency generation microscopy

Despite the old adage "a good craftsman never blames his tools," the benefits of high quality equipment cannot be overstated, particularly with regard to innovation.

Dr. Tessa Calhoun's JDRD team seeks to add equipment to the toolkit of scientists working in the field of nanomaterials by creating a new microscope capable of providing the detailed information necessary to understanding nanoparticle interfacial chemistry.

"Scientists have seen that the properties of nanoparticles seem to be really dependent on their surfaces. By making changes to the surface of the nanoparticle, we can change its properties, specifically those involved in light-producing and charge-carrying," said Calhoun. "There are very small defects on these surfaces called trap states and our goal is to image these directly; thus providing valuable insight about the changes caused by manipulating the nanoparticle surfaces." The results of this imaging could open up an entirely new methodology for studying and characterizing nanoparticles.

Calhoun's microscope will yield an unprecedented glimpse into the chemical environment of nanoparticles and lay the groundwork for future projects with novel and advancing nanomaterials. She intends for the microscope to be made available to scientists from around the world to address a broad range of study in the field of interfacial chemistry.

Qing Charles Cao

Assistant Professor, Department of Electrical Engineering and Computer Science
Science Alliance JDRD - ORNL LDRD 1/1/2015-12/31/2015

Software-defined storage for efficiency and reliability in exascale high-performance computing systems

Countries across the globe are racing toward the creation of the next supercomputer, envisioned as exascale machines that are capable of a million trillion calculations per second. With implications for nearly every field of science and technology, exascale computing has been described as the key to creating and managing a better future.

One key component of exascale computing is fast reading and writing of data using storage systems. In recent years, growing demands for data storage have driven High-Performance Computing (HPC) platforms to adopt a variety of hardware devices as viable storage solutions. However, data processing requirements have also led to more frequent failures, prompting the need for elastic system reconfigurations and failure recoveries.

Cao's JDRD team seeks to address these challenges by creating a software-defined storage layer that can provide flexible, reliable, and elastic storage services and capabilities based on the underlying hardware. Cao proposes that by controlling the way that the storage is configured and data objects are moved across storage tiers, this layer can achieve great improvements on access speed, reliability, and operating cost.

Their first joint paper based on this study between UT and ORNL has been accepted into the International Conference for High Performance Computing, Networking, Storage and Analysis (SC) 2015.

Kimberly Carter

Assistant Professor, Department of Civil and Environmental Engineering
Science Alliance JDRD - ORNL LDRD 1/1/2015-12/31/2015

The use of PFLOTran and uncertainty quantification for modeling subsurface transport of chemical contaminants in hydraulic fracturing wastewater

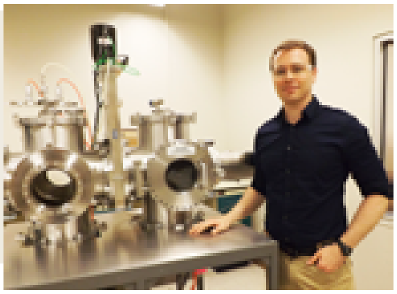
Hydraulic fracturing, or fracking, is a loaded topic these days, given the recent increase in both fracking itself and concerns over its potential impacts. One of the biggest issues surrounding hydraulic fracturing is the environmental impact the industry has on water resources in the United States.

A hydraulically fractured well can require anywhere between two to ten million gallons of water that is then mixed with sand and other chemicals, which can vary in formulation. The injected water returns to the surface as flowback, carrying the chemical additive and shale material which can be benign, toxic or even possibly carcinogenic.

Dr. Kimberly Carter's JDRD team seeks to determine the fate of the chemical constituents in hydraulic fracturing additives. Currently, Carter's team is studying four specific components, though their research has determined that companies conducting hydraulic fracturing have utilized approximately 5,000 different chemicals. In its first year, the project has already discovered that the breaking agent used in fracking, which is intended to prevent water contamination, is ineffective in the small concentrations in which it is currently being applied.

The accompanying LDRD project will address the deficiencies in simulations currently used by the gas and oil industry for evaluating hydraulic fracturing stimulation of production wells.

David C. Donovan



Assistant Professor, Department of Nuclear Engineering
Science Alliance JDRD - ORNL LDRD 1/1/2015-12/31/2015

Plasma-material interaction studies for fusion energy relevant conditions on the ORNL Proto-MPEX device

Plasma-material interaction is one of the most serious technology issues in fusion energy science, and ORNL and faculty members in the Department of Nuclear Engineering at UT have made significant progress in advancing the understanding of this subject.

Dr. David Donovan's JDRD project continues this advancement by supporting a graduate student, Melissa Showers, in working with ORNL's existing equipment to study plasma-material interactions relevant to fusion energy experimental reactors. Showers utilizes an infrared camera to observe the Proto-MPEX device as it exposes sample materials to intense ion damage, experiments which could help predict how damage will occur in fusion reactors.

Showers began the project with very little previous hands on experience with heat flux characterization diagnostics. However, since the beginning of the project, she has learned to perform sophisticated calibrations and has taken data from the experiments that were subsequently presented at group meetings.

The work performed by Showers has proven beneficial to ORNL as the facility lacked the staff to conduct these experiments. Additionally, she will have the opportunity to present her findings at the 57th Annual Meeting of the American Physical Society Division of Plasma Physics Conference, the largest plasma physics conference in the U.S.

Steven Johnston

Assistant Professor, Department of Physics and Astronomy
Science Alliance JDRD - ORNL LDRD 1/1/2015-12/31/2015

Quantum Monte Carlo studies of correlated one-dimensional multi-orbital systems

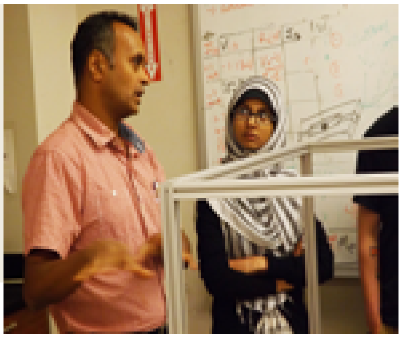
The real world applications of superconductors are practically limitless. For example, recent advances in transportation like magnetically levitating trains, and advances in medical diagnostics are largely based on our knowledge of superconductors.

The recent discovery of superconductivity at high transition temperatures in a class of iron-based materials has prompted a renewed interest in the role of electron mobility and orbital degrees of freedom in superconductivity. Traditionally, high-temperature superconductivity is found when additional electrons are added to an insulating material. However, the new iron based superconductors seem to display a dual nature, where the electrons behave as if they have both localized (insulating) and mobile (conducting) characteristics. Understanding the nature of this duality may hold the key for understanding superconductivity.

Dr. Steven Johnston's JDRD project seeks to explore the underlying physics of these superconductors, with the guiding notion that the selective mobility of electrons is tied to the multi-orbital nature of the pnictides. His team will utilize extensive one-dimensional models in order to study large system sizes to investigate how the mobility of electrons affects factors such as the number of orbitals or the presence of defects in the material.

Ramki Kalyanaraman

Professor, Department of Materials Science and Engineering,
Department of Biomolecular Engineering
Science Alliance JDRD - ORNL LDRD 1/1/2015-12/31/2015



Novel earth-abundant semiconducting oxides and ultrastable bimetals for chemical sensing and energy harvesting

The discovery of a genuine breakthrough in science-based research is not as common as casual observers may think, but Dr. Ramki Kalyanaraman's JDRD team has done just that.

Kalyanaraman's team began their JDRD project by attempting to improve the materials used for optical sensor applications. Currently, the most effective element for these sensors is silver, which unfortunately degrades rapidly once exposed to air, sometimes within a matter of hours. To mitigate this issue, much of the existing technology utilizes gold, which does not perform nearly as well.

Kalyanaraman's JDRD proposal suggested that by combining silver with other metals, including magnetic materials, the integrity as well as performance of the sensor devices could be improved. Indeed, their results have shown that the targeted optical sensor devices made from the combination of materials are much more stable over time as compared to those made from pure gold, and even show better performance. In addition, during these investigations the team made a new and unexpected finding that has culminated in the discovery of a new type of material. This material, which is primarily derived from earth abundant compounds such as iron oxide, could benefit many applications that require semiconductor materials with large optical transparency and large electrical conductivity while also being cost effective by being processable at room temperature.

Kalyanaraman's team is applying this new discovery to optical devices that can convert light into energy as well as for sensing and manipulation of the transmission of light. These new materials are likely to become a core technology in next generation threat assessment for national security purposes.

Nicole McFarlane

Assistant Professor, Department of Electrical Engineering and Computer Science
Science Alliance JDRD - ORNL LDRD 1/1/2015-12/31/2015

CMOS based neutron detection

In the more than 100 years since personal use cameras became widespread, much has changed with the now ubiquitous piece of technology. Gone are the clunky wooden boxes mounted on tripods that sometimes required minutes of stillness from subjects. Cameras are now frequently small enough to fit inside a pocket with blinding shutter speeds and crystal clear resolution.

The goal of Dr. Nicole McFarlane's JDRD team is to do something similar with the neutron detecting cameras currently in use at ORNL.

Neutron detection is a popular imaging method used for a variety of materials, from strands of DNA to chunks of rock. This imaging is currently performed with cameras that use Silicon Photomultiplier (SiPM) chips, which are large and expensive.

McFarlane's team is working to design a prototype that will use Complimentary Metal-Oxide Semiconductor (CMOS) chips, which will lead to smaller, less costly equipment. McFarlane's prototype will be used to determine if the new technology will work as precisely and efficiently as the current SiPM chip equipment. The team sent the first prototype out for fabrication in May, and hopes to complete testing on it in time to commission a second, updated prototype.

Jim Ostrowski

Assistant Professor, Department of Industrial Systems Engineering
Science Alliance JDRD - ORNL LDRD 1/1/2015-4/30/2016

Optimal thermal control in a micro grid

Micro-grids are small-scale power grids that utilize renewable energy sources, such as wind and solar, to create power. With an increasingly taxed power grid supplying the United States with electricity, the micro-grid movement has gained momentum and more and more people are investigating “off grid” living. Unfortunately, the major hurdle with micro-grids in their current state is reliability, as most alternative energy resources are inconsistent.

Ostrowski’s team is investigating methods for improving this reliability by providing a framework for determining an individual grid’s specific requirements, beginning with optimizing thermal control. Thermal load can account for as much as 60% of a building’s consumption of electricity.

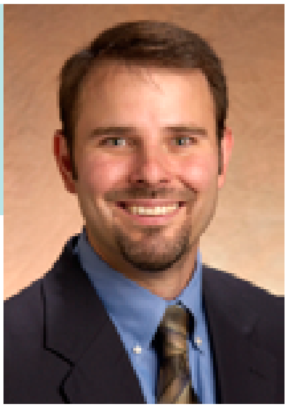
Ostrowski’s team is working on creating a scalable system for determining a thermal schedule that maximizes the reliability of the critical systems while maintaining an optimal outcome. The task becomes far more complex in real-time, when adjustments must be made instantaneously based on ever changing circumstances. Ostrowski’s goal is to create a “warm-starting” technique which can serve as the jumping off point for real-time problem solving.

Micro-grids have potential future applications in a variety of areas, including military posts, refugee camps and aid facilities in the third world. The partnering LDRD project intends to take the Flexible Research Platform building at ORNL off-grid for up to a week at a time, a task Ostrowski’s research will be integral to accomplishing.

Eric Boder

Science Alliance JDRD - ORNL LDRD 1/1/2013-12/31/2014

Domain identification and enzymatic ligation for structural biology of complex proteins



Proteins, life's worker bee molecules, do what's needed to keep cells alive. They play a crucial role in the structure, function, and regulation of living organisms. Often large and complex, life sustaining molecules are composed of multiple stable units called domains, each with a disctinct structure and function; each conserved in near identical form from species to species.

Understanding how they work involves identifying the domains, figuring out what they do, and determining how they fit together - a difficult proposition given the millions of possible arrangements, according to JDRD team leader Eric Boder.

Boder's JDRD team is collaborating with ORNL's Hugh O'Neill to stitch together the structural details of cellulose synthase (CesA) proteins involved in synthesizing plant cellulose. Their goal is to build a tool kit for identifying the structure of extremely complex proteins.

"Individual tags and enzymes that match up with neighboring tags and enzymes will allow us to bring the pieces back together in the proper order," Boder says.

Wei Gao

Science Alliance JDRD - ORNL LDRD 1/1/2013-12/31/2014

User-centric sensing platform for smart buildings

How can we get people to do what we need them to do on behalf of their environment? Incentives.

Smart phones can add to the effectiveness of more expensive built-in sensors in a smart building, tracking readings in temperature, humidity, light, and sound, and configuring the central control units accordingly. Getting smart phone users to help is the trick.

Wei Gao proposes to seamlessly integrate users and their smart phones' sensing capabilities with sensors to greatly improve the accuracy and efficiency of monitoring in smart buildings

Gao's JDRD team's incentives framework makes it possbile for users to participate whether implicitly or explicitly in a flexible, individualized arrangment that minimizes costs and maximizes benefits.

A prototype of the communication and coordination mechanisms required is on track for development, together with a conditioned building system and test bed of users.

Andy Sarles

Science Alliance JDRD - ORNL LDRD 1/1/2013-12/31/2014

Single channel recordings and GISANS of amyloid-beta peptides in fully hydrated, unilamellar lipid bilayers

Cell membranes teach us about how things work in the natural world. Painstaking research decodes the membrane's complex, interacting molecules made up of proteins, peptides, and enzymes. What researchers learn often inspires ideas for practical biomolecular tools or brings clarity about diseases, says JDRD team leader Andy Sarles.

Sarles' JDRD team has singled out cholesterol in the cell membranes of nerve cells in the brain as a possible source for answers about Alzheimer's disease. Cholesterol is prevalent in all cell membranes, Sarles says, most especially in nerve cells (neurons) in the brain.

Sarles' team evaluates the effects Aß peptides have on the permeability of two converging cell membranes that have been synthetically filled with cholesterol molecules.

The team uses a tool Sarles invented to create artificial membranes between two simple water droplets submerged in oil. With it, they can control membrane composition, size, and other properties - historically a difficult task to accomplish.

Tongye Shen

Science Alliance JDRD - ORNL LDRD 1/1/2013-4/30/2015

Coarse-grained modeling of the conformational dynamics of signaling protein complex

Genes may get all the glory, but proteins are where the action is.

Our ability to understand the dynamic motions of proteins is what really counts when we peer into biological systems and observe how they respond to change. Increasingly complex studies of protein systems - as they change shapes to regulate and signal biological processes - hold enormous promise for advances on many research fronts.

In collaboration with ORNL researchers using world-class neutron technology and supercomputing facilities applied to the signaling protein, kinase A (PKA), Shen targets the challenge of studying complex protein systems with a powerful combination of modeling, theoretical, and computational tools.

As a biophysicist, Shen's expertise is grounded in statistical and soft-matter physics and advanced computation. This project gives him the additional opportunity to collaborate in a multidisciplinary study of the large scale, dynamic motions of signaling proteins using the cutting edge technique of small angle neutron scattering (SANS). However, we need better ways to interpret the valuable SANS observations related to flexible, large-scale motions of a signaling protein complex.

Enter Shen's team with "coarse-grained" modeling. The method sacrifices detailed information for the positive advantage of extending both the spatial scale (in terms of size or extent of dynamic motion of the signaling protein) and the time scale. While the calculations are formulated to take less than a few minutes, the approach is sensitive to small perturbations and void of sampling errors.

Wei He

Science Alliance JDRD - ORNL LDRD 1/1/2014-12/31/2014

Understanding and modulating the biocompatability of nanocellulose for advanced biomedical applications

Is nanocellulose toxic? Is nanocellulose stimulatory toward immune cells? Can the biocompatibility of nanocellulose be tuned by chemical modification of its surface?

These are the questions Wei He hopes to answer with her JDRD research. He's project aims to understand and modulate the biocompatibility of nanocellulose for advanced biomedical applications. Nanocellulose, a type of nanomaterial available in abundance and with high renewability, is fueled by its excellent mechanical properties. Nanocellulose has recently made inroads into the biomedical field.

One prominent example is its use in the development of bionanocomposites for tissue engineering and related research.

"Although reports can be found studying the biocompatibility of such bionanocomposites as a whole, few investigated the effects of nanocellulose alone on living cells," He says. "To overcome such a deficit in our understanding of risk pertinent to the use of nanocellulose, a systematic investigation is proposed in this JDRD project, where fundamental studies are designed to reveal the adverse effects, if any, that nanocellulose could pose on living cells grown in a controlled lab setting."

Mingzhou Jin

Science Alliance JDRD - ORNL Seed 1/1/2014-12/31/2014

Stochasting optimization of power management of plug-in electric vehicles

Dr. Mingzhou Jin hopes algorithm development will change the future for plug-in electric vehicles.

Jin's JDRD project helps he and Dr. Andreas Malikopolous at ORNL work together using the Markov Decision Process to model the whole power control diagram of plug-in electric vehicles.

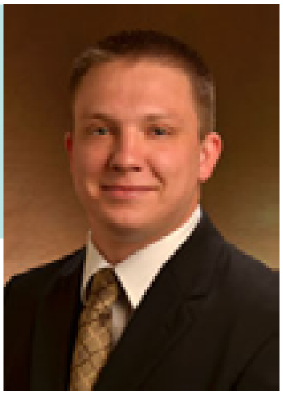
Jin's team, which includes Industrial Engineering Ph.D. students Nelson Granda and Whitney Forbes, has developed the model and is working on the algorithm development.

"The team plans to have a paper draft ready by the end of 2014 and may develop a proposal to the Vehicle Technologies Program (VTP) at the Department of Energy," Jin says.

Eric Lukosi

Science Alliance JDRD - ORNL LDRD 1/1/2014-12/31/2014

Electrical characterization of large area quasi-monocrystalline diamond films



Diamond is a high-powered device's best friend. Eric Lukosi's JDRD research project focuses on the development of a diamond based MESFET device for high power switching applications.

When the current and voltage across a MESFET is large, device self-heating can lead to performance degradation. Diamond has a large band gap and the highest thermal conductivity of any semiconductor, so its application for high power devices shows promise.

However, there are some critical challenges that must be overcome. The most important is the doping of diamond for majority carriers that are vital to device performance and the mobility of these charge carriers in the device, which is related to the device switching speed.

To overcome this challenge, Lukosi's team is investigating the possibility of enhancing the growth of embedded boron delta layers in diamond.

Lukosi said "Creating a true boron delta layer will allow for enhanced device performance and potentially lead to commercial product development and integration."

Stella Sun

Science Alliance JDRD - ORNL Seed 1/1/2014-12/31/2014

Weighted multi-factor authentication through behavior learning

Having a hard time remembering all your passwords? Stella Sun would like to help with that.

Sun's JDRD team is researching multi-factor authentication based on user behavior.

The project proposes a new approach for authentification based on what you do, user behavior, that is implicitly learned by the application. This new approach will be combined with other factors, such as a password, to create multi-factor authentication.

"If successful, this project will fundamentally change user experience for the better, since users do not need to remember a ton of passwords for different applications," said Sun.

Haidong Zhou

Science Alliance JDRD - ORNL LDRD 1/1/2014-12/31/2014

Single crystal growth and neutron scattering studies on new quantum magnets with coexistence quantum spin states and multiferrocity

Haidong Zhou believes UT has the potential to become a national leader in crystal growth.

With his JDRD project, Zhou aims to build a competitive project to perform single crystal growth and magnetic property studies on quantum magnets through strong collaborative efforts between UT and ORNL.

“Natural science and technology are increasingly governed by quantum phenomena. The understandings of the physical properties of quantum matters have been at the forefront of not only the modern condensed matter physics, but also materials science,” Zhou says.

Zhou’s team hopes to enhance materials research through the UT-ORNL Joint Institute for Advanced Materials (JIAM). In addition, Zhou works closely with other materials scientists to pursue a crystal growth center at the University, which could potentially put UT in a national leading position for crystal growth, and therefore generate more impact on materials research.

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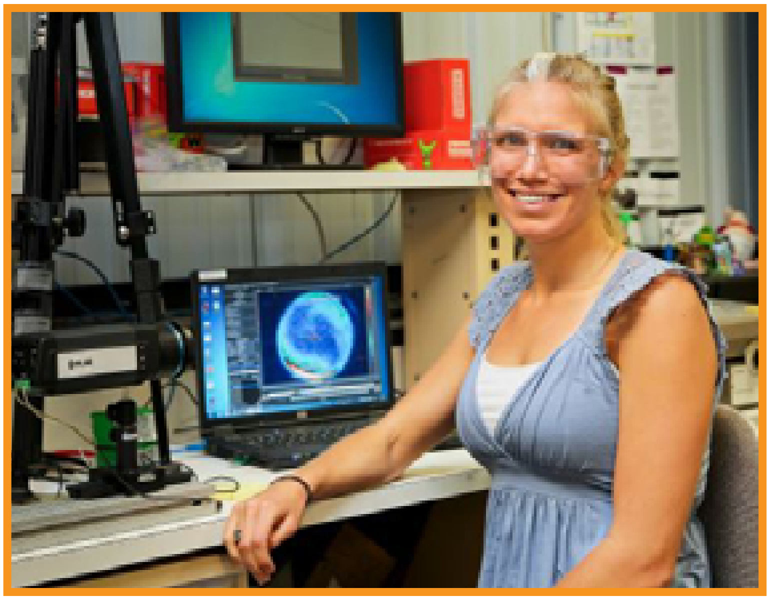
Science Alliance
Student Research & Development



The Science Alliance's Joint Directed Research and Development program has a well-developed evaluation system for proposed projects, which focuses on scientific merit, potential for additional funding and, especially, opportunities for students. Project leaders are encouraged to seek out instances for inclusion of undergraduate and graduate students for mentoring and hands-on experience. As a result, many students have had occasion to add significantly to the foundation of their future careers through direct support provided by JDRD projects.

Graduate student Melissa Showers, via her work with the JDRD project of Dr. David Donovan, has gained a great deal of experience with heat flux characterization diagnostics and the use of infrared cameras while working with scientists and equipment at ORNL. As a result of this research and study, Showers will present her findings at the largest plasma physics conference in the country this fall.

Katherine Manz, a member of Dr. Kimberly Carter's JDRD team, has contributed instrumental research to Carter's project. Manz is credited with determining some of the chemical components in the chemicals used in hydraulic fracturing as well as developing methods for detecting some of these compounds. Additionally, she has functioned as a mentor to two undergraduate students during their research participation.

Dr. Brian Long's team members Kevin Gmernicki and Eunice Hong have been the two primary researchers on Dr. Long's JDRD project. Gmernicki has served as project leader and conducted and overseen all investigations into materials necessary to the design of the team's gas separation membranes. Hong has led all investigations into the synthesis of those materials. Both students have contributed to two publications in progress.

Dr. Tessa Calhoun's graduate student, Brianna Watson, has served as the team's lead student investigator. Working with the JDRD, Watson has built a nonlinear microscope and demonstrated its capability to produce both two-photon fluorescence and second harmonic generation, both of which are necessary steps in the progress of Dr. Calhoun's research. This work led directly to a publication currently under consideration.

Annette Farah, the first year graduate student on Dr. Ramki Kalyanaraman's team, has been working full time on the project. During her time with the JDRD, she has been trained to operate a variety of equipment, including an atomic force microscope, a scanning electron microscope, a broadband optical spectrometer and a thin film depositing system.

Graduate students, postdoctoral researchers and even undergraduate students provide the backbone for much of the research and investigation conducted within the confines of the Science Alliance's JDRD program. Important contributions are made by these scholars to each supported project thereby ensuring the University of Tennessee, as well as the state of Tennessee, a substantial foothold in the future of the nation's scientific community.

Support for Student Education and Research 2014-2015

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. The funds are then disseminated to seven science departments and one engineering department, providing Science Alliance support across a multitude of disciplines and fields of study beyond the narrowed focus of the JDRD program.

The form of this incentivization is based on the best uses to grow the graduate student population in the two colleges. In some cases, it is partial graduate research assistantships, in others it is used for graduate teaching assistantships that lead to graduate research assistantships on federal funded projects in the sciences and engineering. In most cases, these students in the sciences and engineering that are supported have various connections to ORNL: through their advisor's joint faculty status, through ORNL user facilities, and through ORNL advisors on the dissertation committees. Great doctoral programs frequently use central funds to support GTAs for one or two years ahead of GRAs. In the case of Science Alliance funding, all efforts are made to ensure that the connection to ORNL is high.

This year the College of Arts and Sciences received support in the amount of $848,000 and the College of Engineering was given $101,700, for a total of $949,700 in funding distributed to students at the University of Tennessee, Knoxville. This translated into support for 250 students in stipends and fellowships, research, awards and equipment. Subsequently, the supported students have produced dozens of scholarly publications in well-known journals, including the *Journal of Forensic Sciences*, *Journal of Immunology* and *Journal of Physical Chemistry*. Students supported by Science Alliance funds also travelled across the country to give presentations at key conferences in their fields and sought additional support from corporate and governmental resources.

Many of these students are currently being mentored by Science Alliance funded scientists and are actively collaborating with ORNL scientists. They have earned additional funding for their work from a variety of sources, including the U.S. Department of Energy (DOE), the National Science Foundation (NSF), the National Nuclear Security Administration (NNSA) and the Army Young Investigator Program. The table on the following page illustrates the distribution of Science Alliance funds to individual departments in both colleges.

Department	Total Support	Type of Support	Number of Students	Highlights
Biology	$304,540	GTA/GRA	32	More than half of the currently supported students have direct ORNL collaborations or connections. The remainder have potential collaborations or connections with ORNL after they move into their second year. Students have also co-authored 13 total publications and 10 total conference presentations.
Chemistry	159,964	Graduate Student Trainers GTA	13 15	More than 3/4 of supported students are working with mentors with extensive ORNL, National Science Foundation, DOE and and other National Laboratory affiliations. Students have co-authored a total of 14 publications.
Earth & Planetary Sciences	37,225	GTA	9	More than 1/3 of supported students have a supervisor with ORNL collaborations, including Science Alliance Distinguished Scientist Dr. Robert Hatcher. Most students have an ORNL affiliated scientist on their dissertation committee.
Electrical Engineering & Computer Sciences	101,700	GTA/GRA	9	Several students have advisors with previous or current ORNL collaborations, or DOD, DOE, NSF funding.
Geography	10,100	Graduate Student Fellowship	5	More than 50% of supported students have participated in an internship at ORNL, one student has ORNL scientist Dr. Nicholas Nagle as an advisor.
Mathematics	88,857	Fellowship/Stipend	52	More than 50% of supported students have collaborations of their own or via advisors with ORNL scientists, several students are co-advised by and have received grants from ORNL scientists, or completed an internship at ORNL
Physics	237,314	GTA/GRA	32	Nearly half of all supported students have an ORNL connection via the Physics Divisions, the Spallation Neutron Source, or Titan user facilities at ORNL. Most are connected via advisors who are UT based joint faculty, ORNL scientists or have existing collaborations.
Psychology	10,000	GTA	10	Supported students have generated dozens of publication and multiple poster presentations in their chosen area of study. Increasingly, there is more collaboration between UT and ORNL in the neuroscience space.

Collaborative Cohort Program

The Collaborative Cohort Program, introduced by Science Alliance in the fall of 2013, is a two year program designed to nurture collaboration between underrepresented UT junior faculty and ORNL junior scientists. Eligible faculty members include those within ten years of their initial appointment at UT who are working within the STEM disciplines, with a focus on underrepresented groups as defined by UT (e.g., women and ethnic/racial minorities, veterans and individuals with disabilities). Cohort members from UT will work closely with the newly established ORNL Liane B. Russell Fellows.

In 2013, Oak Ridge National Laboratory (ORNL) introduced the Liane B. Russell Fellowship, named after Dr. Liane Russell to honor her groundbreaking research in genetic science. This highly competitive fellowship recognizes and promotes diversity across all fields of research relevant to the missions of ORNL and the U.S. Department of Energy (DOE). A select number of fellowships are awarded annually to candidates who have shown outstanding potential to conduct research of the highest quality and impact. The Russell Fellowship provides funding support for three years, along with formal mentorship to facilitate successful integration of Russell fellows' research with DOE programs and long-term careers with ORNL.

As a whole, the Collaborative Cohort is focused on enabling discovery and scholarly development, collaboration, team building, graduate student mentoring, and obtaining funding from a variety of sources, including other Science Alliance programs, such as the JDRD, ORNL and DOEprograms. The entire cohort convenes a minimum of six times per year at ORNL for site visits, introductions, meetings, planning and mentoring.

Tessa Burch-Smith

Assistant Professor, Biochemistry, Cellular & Molecular Biology

Development of a reverse genetic system for studying gene function in Crassulacean acid metabolism (CAM) plants

Photosynthesis is vital to life, and Tessa Burch-Smith is working to engineer crop plants to perform that process even more efficiently. Crassulacean acid metabolism, also known as CAM photosynthesis is a process employed by plants in the Crassulaceae family, which includes many succulents and dessert dwelling plants.

Burch-Smith's Collaborative Cohort project is working in conjunction with Dr. Xiaohan Yang, a staff scientist at ORNL. Dr. Yang is investigating the molecular mechanisms behind CAM photosynthesis.

CAM photosynthesis is found in plants that grow in areas with limited water availability, which makes it attractive for scientists seeking to engineer important crops that thrive under those conditions. Dr. Yang's team members are using their considerable resources to identify key genes that regulate CAM photosynthesis in the Kalanchoe species.

However, once a gene is identified as important, its function has to be tested to demonstrate its importance. Through the Collaborative Cohort program, Burch-Smith will be developing a system to facilitate the study of gene functions by adapting the Tobacco rattle virus virus-silencing system for use in Kalanchoe. The virus-silencing system takes advantage of a plant's natural antiviral RNA interference responses to remove the RNA encoded by a gene of interest, effectively knocking down or silencing the expression of that gene.

"By the end of the project I hope to have developed a pipeline for silencing Kalanchoe genes of interest and assessing their roles in CAM photosynthesis," Burch-Smith says.

Tessa Calhoun

Assistant Professor, Chemistry

Rapid-scanning transient absorption of heterogeneous micro-environments

Flourescence based microscopy has proven to be a powerful tool for observing the localization of biological species.

However, Tessa Calhoun says it is imperative that we extend these studies to investigate the effect of the local, heterogeneous environment.Transient absorption microscopy (TAM) uses multiple, ultrafast laser pulses to measure the properties and dynamics of a molecule's excited states, which are susceptible to the electron density of its immediate chemical surroundings.

Calhoun's Collaborative Cohort project focuses on advancing TAM instrumentation with a supercontinuum probe, pulse shaping techniques, and rapid scanning capabilities to monitor the location and ultrafast dynamics of molecules as they interact with the membranes of living cells.

Calhoun's work with microscopy has also led to her participation in a pilot project supported by the U.S. Department of Energy's Office of Biological Environmental Research. In a collaboration with ORNL scientists and academics from across the country, her project seeks to develop an adaptive approach to imaging, which will serve as a framework for designing and implementing bioimaging experiments for an array of processes.

Joshua Sangoro

Assistant Professor, Chemical and Biomolecular Engineering

Structure-morphology-property relationships in polymerized ionic liquids

The rising energy needs of modern society continue to provide significant impetus for extensive research and development in energy storage devices. Polymer electrolytes play a key role in these devices.

Polymerized ionic liquids are a new class of polymer electrolytes that exhibit both the outstanding mechanical characteristics of polymers and unique physic-chemical properties of molecular ionic liquids in the same material.

"They have shown remarkable advantages when employed in dye-sensitized solar cells, lithium batteries, actuators, field-effect transistors and electrochromic devices," Sangoro says. "Despite their prospects as ideal polymer electrolytes, the key structure-morphology-property relationships in polymerized ionic liquids are not yet understood."

The goal of Sangoro's Collaborative Cohort project is to obtain a fundamental understanding of the impact of molecular structure, morphology and dynamics on charge transport in polymerized ionic liquids. Sangoro hopes details of the underlying mechanisms of ion transport in polymerized ionic liquids will be unraveled by complementing results from broadband dielectric spectroscopy with insight from the proposed neutron scattering, dynamic-mechanical spectroscopy, NMR and calorimetry experiments.

The experimental data obtained from Sangoro's Collaborative Cohort project has led to one proposal submitted to the Army Research Office. The support from Science Alliance within the framework of this project was instrumental in enabling Sangoro to win a $348K single-investigator grant from the National Science Foundation in May 2015.

Stephanie TerMaath

Assistant Professor, Mechanical, Aerospace and Biomedical Engineering

Supercomputing for multi-disciplinary optimization of obstructed ventricular catheters

Stephanie TerMaath's Collaborative Cohort project could provide relief for the disabled.

TerMaath's project focuses on brain shunts, which are used to treat disabled patients suffering from a range of life-threatening disorders. These disorders include congenital pediatric hydrocephalus, which is the accumulation of spinal fluid in the brain and is present in 1 in 500 live births.

While there is typically no cure for these patients, placement of a brain shunt often leads to symptom relief and prevents brain damage and death. Unfortunately, the brain shunt failure rate is currently greater than 50%, resulting in multiple brain surgeries in a patient's lifetime.

One of the primary causes of failure and reoperation is obstruction of the ventricular catheter, the tube which diverts cerebrospinal fluid from the ventricles to the shunt valve. Improved design and optimization of the ventricular catheter requires the integration of science from the multi-disciplinary fields of high performance computing, fluid dynamics, structural mechanics, materials science, nuclear imaging, mathematics and probabilistic analysis.

TerMaath says, "This project merges scientific knowledge from these diverse fields to advance basic science in order to develop an improved design for ventricular catheters."

UT - ORNL Joint Institutes

Five UT-ORNL joint institutes link distinct, complementary resources in select, high-priority scientific and engineering fields at the University of Tennessee, Knoxville, and Oak Ridge National Laboratory. Each opens doors to leadership-class research instrumentation and computing facilities; offers an environment conducive to collaboration; and provides the physical space where scientists and engineers can exchange ideas and work collectively to answer complex research questions.

UT-ORNL Joint Institute for Advanced Materials

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

UT-ORNL Joint Institute for Biological Sciences

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

UT-ORNL Joint Institute for Computational Sciences

The Joint Institute for Computational 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 Department of Energy National Center for Computational Sciences (NCCS) and UT's National Institute for Computational Sciences (NICS).

UT-ORNL Joint Institute for Nuclear Physics and Applications

The Joint Institute of Nuclear Physics and Applications (JINPA) 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.

UT-ORNL Joint Institute for Neutron Sciences

The Joint Institute for Neutron Sciences (JINS) promotes worldwide neutron scattering collaboration among researchers in biological and life sciences, energy sciences, polymer science, condensed matter physics, and computational sciences.

Simpson Named New JIBS Director

Dr. Michael Simpson, Professor of Materials Sciences and Engineering, Oak Ridge National Laboratory Corporate Fellow, and Group Leader of the Nanofabrication Research Laboratory Group in the Center for Nanophase Materials Sciences (CNMS) at ORNL, has been appointed the next director of the UT-ORNL Joint Institute for Biological Sciences (JIBS). This appointment is in addition to his role at CNMS.

Simpson, an expert in stochastic processes in gene expression, nanobiosciences, and synthetic biology, is a Fellow of the American Association for the Advancement of Science, the Institute of Electrical and Electronics Engineers, and the American Institute for Medical and Biological Engineering, and is a member of the JIBS Advisory Board. His appointment began October 20, 2014.

"This is a special opportunity for me to focus on building thought leadership around solving grand challenges in this fascinating area of complexity in biological systems," said Simpson. "Between the two institutions, we have significant resources in both research talent and exceptional facilities that can be leveraged to achieve scientific excellence. I see many opportunities that align with the ideas that I have heard from both UT and ORNL. It will be exciting to collaborate and get going."

Dr. Martin Keller, Associate Laboratory Director for Energy and Environmental Systems at ORNL, said, "This is a special time in the biological sciences for DOE and other federal agencies and for the desire to solve these grand challenges. We hope to see JIBS become the premier thought leader in this space and leverage the opportunities that exist at ORNL and UT. I am delighted to work with Mike as we move forward."

Tennant Named Director of JINS

Alan Tennant has been appointed director of the Joint Institute for Neutron Sciences at the Department of Energy's Oak Ridge National Laboratory. The institute is a partnership between ORNL and UT.

"Neutrons are the future in characterizing materials, especially soft matter," said Taylor Eighmy, vice chancellor for research and engagement. "With Alan as director, we can begin to establish deep thought leadership at UT and ORNL in this growing field."

Tennant assumes the directorship from Takeshi Egami, the founding director of JINS, who is stepping down after leading the institute for eleven years. Egami will remain as director emeritus as he continues to hold his distinguished scientist position at ORNL and teach at the university.

"I am grateful for Takeshi's leadership as the founding director of JINS and I look forward to working with Alan as he continues to propel neutron science at the institute," Eighmy said.

Tennant brings rich neutron science experience to his new role. Before conducting postdoctoral research at ORNL in the late 1990s, Tennant studied physics at the University of Edinburgh, Scotland, and earned his PhD at the University of Oxford. He served as a professor at the Technical University, Berlin, and institute director in the field of magnetism at the Helmholtz Center Berlin.

Tennant, who serves as a joint faculty member in physics and astronomy, continued, "It isn't only about engaging PhD students, but faculty, too. JINS should be a place for both to come and learn more about neutrons, to hold workshops and courses. Science is moving very quickly, and our staff and faculty need to develop along with it. JINS provides a way for both ORNL and UT to engage and perform at the very leading edge of science. With this I think it's possible to do absolutely groundbreaking research that might not happen otherwise."

New NSF Award Supports Continued Operations at JICS

The Joint Institute for Computational Sciences (JICS), a partnership between UT and Oak Ridge National Laboratory (ORNL), has received $3 million in new funding from the National Science Foundation (NSF) to continue to provide advanced computing resources through July 2016. The NSF award covers management and operation of machines called Darter and Beacon.

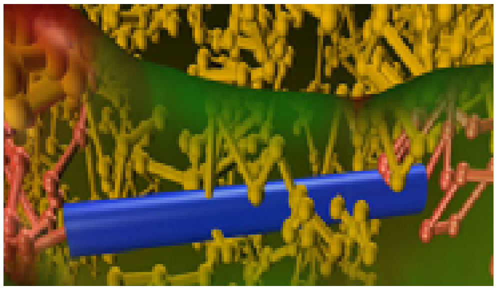
"By virtue of this award to sustain advanced computing resources for a wide spectrum of researchers across the country, JICS is also able to make available these same resources to UT researchers," said JICS director Tony Mezzacappa.

"Darter and Beacon are diverse and powerful and yet easy to use. They can support not only research in the physical sciences but also in other disciplines, such as the social sciences. The resources we maintain are capable of meeting a variety of needs: high-performance computing (HPC), large-memory computing, high-throughput computing, and more."

The National Institute for Computational Sciences, one of NSF's national advanced computing centers and operated by JICS, deploys Darter.

The machine has a peak performance of 240.9×10^{12} (approximately 241 trillion) floating-point operations per second. One floating-point operation is the equivalent of multiplying, adding, subtracting, or dividing two fifteen-digit numbers.

Darter is housed at ORNL near Titan, the second most powerful computer in the world.



"Darter can be used as an HPC platform, where one uses the whole platform for one job, or as a high-throughput computing platform, where one runs many smaller jobs at once," said Mezzacappa. "It can also fulfill an intermediary role toward running on resources designed for the largest computing jobs, such as Titan, the second most powerful computer in the world, and Summit, the third evolution of ORNL's supercomputers, set to come online in 2017."

Beacon is a very powerful, versatile computing cluster that uses traditional central processing units and Intel Xeon Phi coprocessors. Such coprocessors can perform certain kinds of computations very quickly, thereby "accelerating" many different applications. Equally important, Beacon provides a large amount of memory to the computations performed on it, making it well suited to meet the needs of users with large-memory computing jobs.

From a human perspective, JICS houses a number of computational scientists, who are science and engineering domain experts, across a broad range of domains. They serve as an ideal bridge between researchers and the resources. The remaining staff members within JICS provide the foundational support necessary for users and the facility.

"In its accelerated efforts to engage UT campus, JICS has already helped a number of research groups," said Mezzacappa. "The combination of advanced computing resources and a national-class staff of experts has been greatly enabling for researchers on campus with whom we've collaborated.

"My experience is that everyone on the UT campus who relies on computing for research can benefit from what JICS has to offer. My hope is they will come to us so we can bring our significant resources and expertise to bear on their work. Everyone, at all levels of computing and for all types of computing, can benefit from advanced computing. We need to demolish the stereotypes that have kept people away from taking advantage of JICS."

NICS National Institute for Computational Sciences

Oak Ridge National Laboratory

Institute for Advanced Composites Manufacturing Initiative

The Shelby Cobra, a fully electric vehicle 3-D printed at Oak Ridge National Laboratory's Manufacturing Demonstration Facility, was displayed at the 2015 Orange and White Game at Neyland Stadium Saturday, April 25. More than 60,000 people attended the game and had the opportunity to get an up-close view of IACMI's capabilities. University of Tennessee, Knoxville Chancellor Cheek, ORNL researcher Randy Lind and former Vol Bruce Wilkerson posed for a photo with the car.

In January 2014, a new National Network for Manufacturing Innovation (NNMI) Institute was announced and the University of Tennessee, Knoxville was chosen to lead a consortium of universities partnering with the Oak Ridge National Laboratory to establish the Institute for Advanced Composites Manufacturing Initiative (IACMI). The Composites Institute represents $259 million dollars of public-private investments for the next five years to rapidly develop low cost carbon fiber composites for automotive, wind energy, and compressed gas storage markets.

IACMI is operated by Collaborative Composites Solutions (CCS) Corporation as a 501(c)(3) subsidiary of the UT Research Foundation. The university and the UTRF have leadership roles in the governance board of CCS. Further, this is just one of three NNMIs that UT is involved in nationally, with roles also in America Makes and LIFT (Lightweight Innovations for Tomorrow). Advanced manufacturing—critical to the Tennessee economy—is a cornerstone of an important collaboration between UT and ORNL.

Dr. Dayakar Penumadu, Fred N. Peebles Professor and Joint Institute for Advanced Materials (JIAM) Chair, serves as the Characterization Fellow for IACMI (www.iacmi.org) and also as the chief scientist for the institute work conducted at UT. In fiscal year 2015, Science Alliance allocated $88,000 in seed funds for Penumadu to work toward developing low-cost carbon fiber for composites. These funds are distributed on a cost-sharing basis with IACMI. The use of Science Alliance funds enables at least a 1:1 cost share from federal dollars and 1:1 cost share from private sector partner dollars on these projects. Current private sector partners include Ford, Dow, DowAksa, Strongwell, TPI, and GE.

Penumadu's work on evaluating multi-scale mechanical properties of single carbon fibers all the way to multi-laminates using a new class of low cost carbon fiber materials, leveraging unique resources of the U.S. Department of Energy available through the Carbon Fiber Technology Facility here in Oak Ridge. Low cost carbon fibers will also dramatically change the landscape of their use in additive manufacturing (3-D printing) and will pave the way for light weighting requirements for transportation sector. He is leveraging the unique resources available through IACMI's mechanical characterization facilities, JIAM's advanced electron microscopy and x-ray diffraction resources, and the Joint Institute for Neutron Science's (JINS) neutron scattering and imaging facilities for his and his collaborators ongoing research on exploiting the next generation composite manufacturing techniques and educational integration.

The 2014-2015 Annual Report is a publication of the Science Alliance,
a Center of Excellence at the University of Tennessee.

This report is published for the Tennessee Higher Education Commission.

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Publication #: R01-1001-051-001-16