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.

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Vice Chancellor for Research & Engagement
Taylor Eighmy
Associate Vice Chancellor for Research Development
Janet Nelson

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Accounting Specialist II Missy Hodge

Science Alliance Span of Operation
July 1984–2014
Dear Colleagues:

The Science Alliance investment is fundamental to the partnership between the University of Tennessee, Knoxville and Oak Ridge National Laboratory (ORNL). Over time, this relationship has grown and now reflects the diversity of engagement between our two institutions: extensive collaborative research and development; five joint institutes; approximately 145 joint faculty members; 15 governor’s chairs; six distinguished scientists; annual support through the jointly-directed research and development (JDRD) program; the Bredesen Center; the Graduate School in Genome Science & Technology; several appointments to common advisory councils and boards; and an expanding corporate engagement strategy.

New to our Science Alliance program this year is the Liane Russell JDRD Faculty Cohort Program. Dr. Liane Russell, a renowned mammalian geneticist at ORNL, DOE Enrico Fermi Award winner, and member of The National Academy of Sciences, served as a pioneer for women in the sciences during her illustrious career. Established in advance of the ORNL Liane Russell Early Career Fellows, this program brings four UT faculty members into a cohort-mentoring program with the lab’s three Liane Russell Fellows. All seven cohort members will be mentored by faculty and senior scientists, the UT Office of Research & Engagement and ORNL, and DOE participants so as to further advance their research careers.

Our faculty selected in this first cohort are Dr. Tessa Burch-Smith, assistant professor of biochemistry and cellular and molecular biology; Dr. Tessa Calhoun, assistant professor of chemistry; Dr. Joshua Sangoro, assistant professor of chemical and biomolecular engineering; and Dr. Stephanie TerMaath, assistant professor of civil and environmental engineering (see http://tiny.cc/tntoday-scialli and http://tiny.cc/ornl-scialli).

We look forward to the progress that the entire cohort will make as they further their collaborations and growth as scientists and engineers.

Best regards,

Taylor Eighmy
Vice Chancellor for Research & Engagement
University of Tennessee, Knoxville
Overview

The Science Alliance, a Tennessee Center of Excellence established in 1984 and supported annually by the Tennessee General Assembly, has a mission to expand collaboration in research and development with ORNL so as to enhance science and engineering research programs at the University of Tennessee (UT).

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. They are also used to support jointly developed research and development (JDRD) between university faculty and students and ORNL, and ORNL’s efforts to invest in research through their laboratory-directed research and development (LDRD) funding. Finally, funds are used to support graduate student education in the sciences and engineering at UT.

The investment made by the state each year in this important collaboration is both welcome and appreciated. It serves a critical role in leveraging the federal investments made at ORNL and UT in our areas of collaborative research and development.
Distinguished Scientist Program

The Distinguished Scientist Program supports high profile, internationally recognized leadership appointments in science and engineering. The program anchored the Science Alliance partnership-building role during the center’s early years. Appointees were recruited to joint UT-ORNL positions as tenured distinguished UT professors and senior ORNL research staff. Since 2005, joint appointments at this level have been made through the Governor’s Chair Program.

Elbio Dagotto
Nanoscale dimensions and correlated electronic behavior
UT Department of Physics and Astronomy;
ORNL Division of Materials Science and Technology

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.

Takeshi Egami
Atomic-scale dynamics of liquids and glasses; High-temperatures superconductivity
UT Departments of Materials Science and Engineering and Physics and Astronomy;
ORNL Division of Materials Science and Technology

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

Georges Guiochon
Separation Science
UT Department of Chemistry

Georges Guiochon is an expert in using multidimensional chromatography to separate the components of complex samples. His research improves the efficiency of chromatographic columns, optimizes conditions for maximum production rate of safe and effective pharmaceuticals, and examines the complex fundamentals of supercritical fluid chromatography.

Robert Hatcher
Structural geology and tectonics of continental crust
UT Department of Earth and Planetary Science

A structural and tectonics geologist, Robert Hatcher studies the processes that create and evolve Earth’s continental crust.
David Joy
Accurate microscopic and nanoscale imaging
UT Departments of Biochemistry and Cellular and Molecular Biology and Materials Science and Engineering; ORNL Division of Materials Science and Technology

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 ultimately could offer direct, high-resolution imaging at subatomic and subnanometric scales.

Joseph Macek
Electron vortices in simple atomic systems
UT Department of Physics and Astronomy

The probabilities 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.

Jimmy Mays
Synthesizing new polymer membranes for fuel cells
UT Department of Chemistry; ORNL Division of Chemical Sciences

Jimmy Mays synthesizes new, precisely tailored polymers and examines their molecular architecture, composition, and blending capability to discover how form and structure, including their nanonstructural order, might be manipulated to create useful materials.
The table that follows 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. Several examples follow.

**Elbio Dagotto**
Principal investigator of the Field Work Proposal (FWP) titled “Theoretical Studies of Complex Collective Phenomena” that supports the work of two ORNL staff members (R. Fishman and S. Okamoto) and two joint faculty with UT (E. Dagotto and A. Moreo).

Continued inclusion in list of most Cited Physicists. Hirsh index is 65, and number of citations exceeds 20,000.

**Takeshi Egami**
Principal Investigator on the ORNL Field Work Project Atomistic Study of Bulk Metallic Glasses.

Recipient of the J. D. Hanawalt Award.


**David Joy**
In conjunction with Drs. Brian Anderson, and Adam Rondinone at ORNL, designed and built a “Time of Flight Secondary Ion Mass Spectrometer” In conjunction with the helium ion microscope, this project, if successful, will make possible chemical microanalysis on a scale at least one order of magnitude more sensitive then any existing tool, and have a factor of 3 to 5 times better spatial resolution.

In conjunction with Subhadarshi Nayak, has received second and third year support from USDOE to design and demonstrate a digital secondary electron detector system. This program is now funded in total to about $800,000 and will support research at UTK.

**Jimmy Mays**
Involved in Polymer Based Multi-component Materials project, an ORNL FWP led by Alexei Sokolov, which is funded at $2M per year.

Recipient of Bill & Melinda Gates Foundation Grand Challenges Explorations Award.
<table>
<thead>
<tr>
<th>Prin Inv</th>
<th>Project Name</th>
<th>Project Title</th>
<th>Start Date</th>
<th>End Date</th>
<th>Award Amount</th>
<th>FY 14 Expenditures</th>
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<td>09/30/2013</td>
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<td>Computational Studies of Model Hamiltonians for Phases and Multiferroic Manganites</td>
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<td>NRC-HQ-11-G-04-0085 Hatcher</td>
<td>Two-Year Collaborative Research Project to Assess Large Earthquake Seismology in the ETSZ</td>
<td>09/26/2011</td>
<td>09/25/2015</td>
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<td>Detailed Geologic Mapping of Quaternary French Broad River Terraces, Eastern Tennessee</td>
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<td>04/30/2014</td>
<td>8,217</td>
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<td>Geologic Mapping of the Lancing, Hebbertsburg, and Po Creek 7.5 minute quadrangles, Wild and Scenic River</td>
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<td>03/31/2015</td>
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<td>Electron Microscopy Facility</td>
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<td>SRC-2011-OJ-2122 Joy</td>
<td>Focused Helium Ion Beam Induced Synthesis for Repair, Metrology Sample Preparation, and Lithography</td>
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<td>Theory of Atomic Collisions and Dynamics 12 49%</td>
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<td>Collaborative Research: Synthesis and Rheology of Strategically Designed Long-Chain-Branched Polymers</td>
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<td>Fundamentals of Ionic Conductivity in Polymeric Materials for Energy Storage Applications: How to Decouple Ionic Motions from Segmental Dynamics</td>
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<td>08/31/2013</td>
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<td>TN Solar Conversion and Storage Using Outreach, Research and Education (TN-SCORE)</td>
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<td>Nanofiller Reinforced Nonwoven Sandwiched Composites</td>
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<td>Improved Carbon Nanotube Fibers through Crosslinking and Densification</td>
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<td>PFI-BIC: Superelastomers: New Thermoplastic Elastomers Based on Multigraft Copolymers</td>
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<td>Mays</td>
<td>Bill &amp; Melinda Gates Fnd OPP1098281 Mays</td>
<td>Ultra-Sensory Condoms Based on New Superelastomer Technology</td>
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Total External Funds $7,840,526 $2,437,444

Total Distinguished Scientist ORNL Match $1,085,982 $992,948
Joint Directed Research and Development

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

A dual UT and ORNL venture, JDRD complements the Laboratory Directed Research and Development program (LDRD) at ORNL. 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 JDRD program identifies and supports corresponding areas of research at the University of Tennessee, Knoxville. Projects approved for the program have both a University of Tennessee and an Oak Ridge National Laboratory component.

JDRD awards run for two 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 FY2014, Science Alliance funded eight first year JDRD projects and four second year projects.

Eric Boder
Associate Professor, Chemical and Biomolecular Engineering
JDRD project (second year):
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.
Joint Directed Research and Development Program

Often large and complex, life-sustaining molecules are composed of multiple stable units called domains—each with a distinct structure and function; each conserved in near identical form from specie to specie.

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, says JDRD team leader Eric Boder.

Boder has a JDRD team which 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
Assistant Professor, Electrical Engineering and Computer Science
JDRD project (second year):
User-centric sensing platform for smart buildings

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

Smart phones can add to the effectiveness of more expensive built-in sensors in a smart buildings—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.
Joint Directed Research and Development Program

Gao’s JDRD team’s incentive framework makes it possible for users to participate either implicitly or explicitly in a flexible, individualized arrangement 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
Assistant Professor, Mechanical, Aerospace, and Biomedical Engineering
JDRD project (second year):
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 Aβ 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
Assistant Professor, Biochemistry and Cellular and Molecular Biology
JDRD project (second year):
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 experimenters using world-class neutron technology and supercomputing facilities applied to the signaling protein, kinase A (PKA), Tongye 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.
Daniel Costinett  
Assistant Professor, Electrical Engineering and Computer Science  
JDRD project:  
Targeted Drive Train DC-DC Design for Electric Vehicles Using Additive Manufacturing and Wide Bandgap Semiconductors

JDRD funding could improve the performance of hybrid electric vehicles.
Daniel Costinett’s project will leverage previous and ongoing efforts at ORNL in order to achieve a reconfigurable, integrated, efficient, and low-cost DC-DC power converter for plugin and hybrid electric vehicles.

Using recent technological advances in additive manufacturing and wide bandgap semiconductor materials, coupled with a reimagining of the approach to the design of power electronics, the proposed project will demonstrate a DC-DC converter which is both 25% smaller and 40% lower cost than the state-of-the-art, all while reducing total energy losses by 30%.

It is expected that the system advances resulting from this collaboration will yield a breakthrough in the electric vehicle cost-performance ratio and facilitate future collaboration between the UTK and ORNL teams.

Wei He  
Associate Professor, Materials Science and Engineering  
JDRD project:  
Understanding and Modulating the Biocompatibility of Nanocellulose for Advanced Biomedical Applications

Is nanocellulose toxic? Is nanocellulose stimulatory toward immune cells? And can the biocompatibility of nanocellulose be tuned by chemical modification of its surface? These are the questions Wei He hopes to answer with his JDRD research.

He’s project aims to understand and modulate the biocompatibility of nanocellulose for advanced biomedical applications.

Nanocellulose, a type of nanomaterials of natural origin with great abundance and 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 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.”
Joint Directed Research and Development Program

Mingzhou Jin
Associate Professor and Associate Head, Industrial and Systems Engineering
JDRD project:
Stochastic 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 Malikopoulos 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.

Brian Long
Assistant Professor, Chemistry
JDRD project:
Tailored Synthesis of Complex Polymeric Membranes for Carbon Dioxide Purification

According to the US Environmental Protection Agency, in 2011, approximately 6,702,000,000 metric tons of carbon dioxide (CO2) were released into the Earth’s atmosphere as a result of fossil fuel combustion for electrical energy generation and transportation.

In an effort to decrease these emissions, Brian Long’s JDRD project has targeted the development and utilization of polymeric membranes that provide efficient separation of CO2 from other non-greenhouse gases.

Long’s team is focusing on the synthesis, fabrication, and characterization of polymeric membranes that simultaneously maximize permeability and selectivity for CO2 separations.

Specifically, they have developed and thoroughly investigated a class of highly rigid yet highly porous polymers that contain CO2-philic, or CO2 loving functionalities. These polymers have demonstrated remarkable CO2 separation ability and have provided foundational insight into the team’s ongoing and future membrane development efforts.
Eric Lukosi
Assistant Professor, Nuclear Engineering
JDRD project:
Electrical Characterization of Large Area Quasi-Monocrystalline Diamond Films

Diamond is a high power 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 leads to performance degradation. Diamond has a large band gap and the highest thermal conductivity of any semiconductor, so its application for high power devices show 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
Assistant Professor, Electrical Engineering and Computer Science
JDRD project:
Weighted Multi-Factor Authentication through Behavior Learning

Have 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 authentication, based on what you do (or 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,” Sun says.
Joint Directed Research and Development Program

Haixuan Xu
Assistant Professor, Materials Science and Engineering
JDRD project:
Transport Properties of Interfacial Defects in Materials

Haixuan Xu hopes to continue an initiative started by the White House. His JDRD project is focused on computational design of materials to achieve desired properties, which follows the paradigm of Materials Genome Initiative (MGI) started by the White House and currently sponsored by multiple funding agencies.

This research is an effort to build a strong representation of MGI-related research in advanced materials, which enhances not only the UT/ORNL relationship but also the preparedness of UT’s research portfolio in MGI.

In particular, this project is going to examine the defect transport properties of a large number oxide superlattice using high-throughput first principles calculations, which is the key software infrastructure to carried out MGI research and will be applicable to a wide range of materials issues.

“What I really hope to accomplish is to strategically position UT and ORNL for future research endeavors within the Materials Genome Initiative (MGI) and the Integrated Computational Materials Engineering,” Xu says.

Xu hopes the capabilities developed by his project will attract external funding support for various problems in materials research.

Haidong Zhou
Assistant Professor, Physics
JDRD project:
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 lead the nation for 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 recently formed Joint Institute of the Advanced Materials (JIAM). In addition, Zhou works closely with other materials scientists to pursue a crystal growth center at the university, which potentially will put UT in a leading position in the nation for crystal growth and therefore generate more impact on materials research.
UT Science Alliance Collaborative Cohort Program

Tessa Burch-Smith
Development of a reverse genetic system for studying gene function in Crassulacean metabolism (CAM) plants
Department of Biochemistry and Cellular and Molecular Biology
College of Arts & Sciences

Tessa Calhoun
Rapid-scanning transient absorption imaging of heterogeneous micro-environments
Department of Chemistry
College of Arts & Sciences

Joshua Sangoro
Structure-morphology-property relationships in polymerized ionic liquids
Department of Chemical and Biomolecular Engineering
College of Engineering

Stephanie TerMaath
Supercomputing for multi-disciplinary optimization of obstructed ventricular catheters
Department of Civil and Environmental Engineering
College of Engineering
Collaborative Cohort Program

The Collaborative Cohort Program, a new effort introduced by Science Alliance in Fall 2013, will nurture collaboration between underrepresented UTK junior faculty and ORNL junior scientists. Cohorts from UTK will work closely with the newly established ORNL Liane B. Russell Fellows. The focus for the cohorts will be on enabling discovery and scholarly development, collaboration, team building, graduate student mentoring, and the obtaining of funding from a variety of sources, including UTK JDRD, ORNL Laboratory-directed R&D (LDRD), DOE and other funding organizations.

Tessa Burch-Smith
Assistant Professor, Biochemistry, Cellular & Molecular Biology
Cohort Project:
Development of a reverse genetic system for studying gene function in Crassulacean acid metabolism (CAM) plants

Photosynthesis is a vital process, and Tessa Burch-Smith is working to engineer crop plants to perform that process even more efficiently. Burch-Smith is collaborating with Dr. Xiaohan Yang, a staff scientist at ORNL. Dr. Yang is investing the molecular mechanisms behind crassulacean acid metabolism (CAM)-type 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 crop plants to perform photosynthesis under those conditions. Dr. Yang’s group has considerable bioinformatics, genomics and proteomic resources and they are using those to identify key genes that regulate CAM photosynthesis in 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 (TRV) virus-silencing (VIGS) system for use in Kalanchoe. VIGS 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 the effects on CAM photosynthesis,” Burch-Smith says.

Tessa Calhoun
Assistant Professor, Chemistry
Cohort Project:
Rapid-Scanning Transient Absorption Imaging of Heterogeneous Micro-Environments

Fluorescence-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.

**Joshua Sangoro**  
Assistant Professor, Chemical and Biomolecular Engineering  
Cohort Project:  
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 physico-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,” Joshua 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 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.

Improved understanding of the link between polymer dynamics and ion transport is of immediate significance to numerous current as well as future technologies and will contribute to energy sustainability.

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.

Improved understanding of the link between polymer dynamics and ion transport is of immediate significance to numerous current as well as future technologies and will contribute to energy sustainability.
The Collaborative Cohort program could provide relief for the disabled.

Stephanie TerMaath’s project is focusing on brain shunts, which are used to treat disabled patients suffering from a range of life-threatening disorders. Those disorders include congenital pediatric hydrocephalus, which is present in 1/500 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. Despite the consequences for patients, brain shunt failure rate is over 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 (CSF) 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, material 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.”
Distinguished Scientists

Elbio Dagotto
ORNL Materials Science and Technology UT Department of Physics and Astronomy


Takashi Egami
ORNL Materials Science and Technology UT Department of Materials Science and Engineering and Department of Physics and Astronomy


Publications – 2013


Georges Guiochon
UT Department of Chemistry


Kamarei, F., Gritti, F., Guiochon, G., “Investigation of the axial heterogeneity of the retention factor of carbamazepine along an


Robert Hatcher
UT Department of Earth and Planetary Science


David C. Joy
ORNL Materials Science and Technology: UTK Department of Biochemistry, Cellular and Molecular Biology & Department of Materials Science and Engineering


He, Q., Joy, D.C., Keffe, D.J., “Impact of Oxidation on Nanoparticle Adhesion to Carbon
Publications – 2013


Jimmy Mays
ORNL Chemical Sciences Division: UT Department of Chemistry


Joint Directed Research and Development Publications

Jens Gregor

ORNL Chemical Sciences Division: UT Department of Chemistry

Kim, F., Penumadu, D., Gregor, J., Kardjilov, N., and Manke, I., “High resolution neutron and x-ray imaging of granular materials,” Journal of Geotechnical and...
Geoenvironmental Engineering. American Society of Civil Engineers (ASCE), 139:715-723 (2013).


David Jenkins
UT Department of Chemistry


Veerle Keppens
ORNL Materials Science and Technology: UT College of Engineering


Ed Perfect
UT Department of Earth and Planetary Sciences

FY14 Support for Student Education & Research

A total of $949,700 of Science Alliance funding is distributed through the College of Arts and Sciences and the Department of Electrical Engineering and Computer Science in the College of Engineering. Arts and Sciences receives $848,000. EECS receives $101,700.

The tables that follow show the distribution of Science Alliance support for graduate and undergraduate education and research in seven science departments and one engineering department at The University of Tennessee, Knoxville.

Table I provides a broad, overall breakdown of the FY14 expenditures in the College of Arts and Sciences. The remaining tables variously list specific individuals, project titles, and the purpose funds served.

### Reported Departmental Science Alliance Expenditures FY14

**College of Arts and Sciences**

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<thead>
<tr>
<th>Expenditure Category</th>
<th>Biology Division</th>
<th>Chemistry</th>
<th>Earth &amp; Planetary</th>
<th>Geography</th>
<th>Mathematics</th>
<th>Physics</th>
<th>Psychology</th>
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<td>5</td>
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<td>$8,131</td>
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**College of Engineering**

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<td>Graduate student stipends/ fellowships</td>
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<td><strong>Biochemistry, Cellular and Molecular Biology Department</strong></td>
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<td>Bucci, Joel</td>
<td>Identifying metal binding sites of plasminogen activator inhibitor-I</td>
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<td>Cooper, Joanna</td>
<td>Inhibiting lipoprotein receptor-related protein 1 with receptor associated protein prevents glutamate-induced phase delays of the SCN circadian clock</td>
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<td>Gahlot, Vandna</td>
<td>Nuclear receptor N-terminal domains.</td>
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<td>Holbrook, Kristen</td>
<td>Biochemical Analysis of the Torsin AAA+ Cycle</td>
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<td>Lokdarshi, Ansol</td>
<td>Investigate the role of CML38 protein in oxidative stress in plants</td>
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<td>Madison, Stephanie</td>
<td>Investigating the role of class XI myosins in pollen tube growth using the model plant Arabidopsis thaliana</td>
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<td>Mukherjee, Tanmoy</td>
<td>Characterizing the contribution of multiple chemotaxis proteins to regulating motility responses in a bacterium. He is using genetic approaches and fluorescence microscopy to characterize the function of these proteins.</td>
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<td>Nair, Sudershana</td>
<td>Working on the regulatory mechanisms of PDF gene expression that controls clock output pathways in the fruit flies.</td>
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<td>Presley, Sarah Nichole</td>
<td>Characterizing the allostery within nuclear receptor ligand binding domains (LBDs).</td>
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<td>Puster, Letitia</td>
<td>Neutron scattering to evaluate protein: protein interactions that regulate protease inhibition and are important for blood coagulation, cancer, and inflammation.</td>
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<td>Rosendall, Kately</td>
<td>NMR experiments with whole cells that expresses one of the aminoglycoside modifying enzymes and cause resistance to the action of several aminoglycoside antibiotics.</td>
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<td>Ryan, Jennifer</td>
<td>Investigation of binding partners of the MYA1 Globular Tail.</td>
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<td><strong>Ecology and Evolutionary Biology</strong></td>
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<td>Austin, Emily</td>
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<td>Bernard, Riley</td>
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<td>Birkebak, Joshua</td>
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<td>Cantwell, Lisa</td>
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<td>Clemmensen, Sharon</td>
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<td>Domoulin, Christine</td>
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<td>Hollingsworth, Phillip</td>
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### Ecology and Evolutionary Biology

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<td>Kim, Jaymelee</td>
<td>Spatial data mismatches responsible for estimation bias when prioritizing areas for protection.</td>
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<td>Sutton, Nathan</td>
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<td>Ward, Shelby</td>
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### Microbiology

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<td>Comparative genomics of G-protein coupled receptors</td>
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<td>Chandler, Jeremy</td>
<td>Relationships among Prochlorococcus ecotypes across oceanic temperature ranges</td>
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<td>Dogra, Pranay</td>
<td>Role of viral chemokines in cytomegalovirus pathogenesis</td>
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<td>Kevorkian, Richard</td>
<td>Geochemical Control of Methanogenesis in Cape Lookout Bight</td>
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<td>Fe-Dependant Denitrification, O2 Detox., and U Reduction by strain 2CP-C</td>
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<td>Environmental Constraints on Cyanomyophage Abundance in the North Pacific Ocean</td>
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<td>Purcell, Alicia</td>
<td>Selection of microbial species and physiologies in extreme environments</td>
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<td>Saito, Holly</td>
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<td>Schwab, Elliot</td>
<td>Examining the impact of mouse virulence phenotype on the global population structure of Toxoplasma gondii</td>
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<td>Smartt, Abby</td>
<td>A Genomic and Transcriptmic Approach to Understanding Cold Acclimation in Pseudomonas fluorescens HK44</td>
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<td>Tams, Robert</td>
<td>The Role of Phosphatidylcholine and DGTS in C. Albicans virulence</td>
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### Awards

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<td>Li, Zhou</td>
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<td>Fong, Jonathan Kelly</td>
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<td>Gan, Yundi</td>
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### Summer Undergrad Program
- Conner, Elizabeth Christina

### Analytical Instrumentation Lab Trainer
- Cramer, Steven Alan

### NMR Lab Trainer
- Dhah, Harkiran K

### Molecular Modeling (SYBYL) Trainer
- Gan, Yundi
Support for Student Education and Research – 2013-2014

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<th>PROJECT TITLE/PURPOSE</th>
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<tr>
<td>Garland, Michelle Epstein</td>
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<td>Gibson, Stephen Colin</td>
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### Support for Student Education and Research – 2013-2014

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39
### Centers of Excellence/Centers of Emphasis
**Actual, Proposed, and Requested Budget**

**Institution:** The University of Tennessee, Knoxville  
**Center:** The Science Alliance

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<th>FY15-16 Requested</th>
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<td><strong>Salaries</strong></td>
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| **Matching**   | **Appropr.**     | **Total**         |
| 1,995,119      | 1,853,725        | 3,848,844         |
| **Total Salaries** | **1,909,337** | **3,848,844**     |
| **1,034,678**  |                  | **1,293,529**     |
| **2,379,941**  |                  | **2,379,941**     |
| **4,166,235**  |                  | **4,166,235**     |

| **Fringe Benefits** | **13,153** | **19,350** |
| **Total Personnel** | **2,513,951** | **2,302,455** |
| **2,371,529** | **1,966,617** |
| **5,214,304** | **4,166,235** |

| **Non-Personnel** | **Travel** | **283,220** | **225,000** | **193,920** |
| **Software** | **13,153** | **19,350** |
| **Books & Journals** | **283,220** | **225,000** | **193,920** | **225,000** |
| **Other Supplies** | **13,153** | **19,350** |
| **Equipment** | **4,369** | **8,739** |
| **Maintenance** | **1,772** | **4,219** |
| **Scholarships** | **119,628** | **56,357** |
| **Consultants** | **0** | **0** |
| **Renovation** | **0** | **0** |
| **Other (Specify)** | **0** | **0** |
| **Prof Services & Memberships** | **21,855** | **6,591** |

| **Total** | **13,153** | **19,350** |
| **2,513,951** | **2,302,455** | **5,214,304** |

| **2,371,529** | **1,966,617** |
| **5,214,304** | **4,166,235** |

| **13,153** | **19,350** |
| **2,513,951** | **2,302,455** |

| **2,371,529** | **1,966,617** |
| **5,214,304** | **4,166,235** |
## Financial Table

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<td>Printing, Duplicating, Binding</td>
<td>2,195</td>
<td>3,766</td>
<td>5,961</td>
</tr>
<tr>
<td>Utilities and Fuel</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Communications</td>
<td>3,223</td>
<td>5,031</td>
<td>8,254</td>
</tr>
<tr>
<td>Computer Services</td>
<td>773</td>
<td>1,316</td>
<td>2,089</td>
</tr>
<tr>
<td>Rentals</td>
<td>413</td>
<td>704</td>
<td>1,117</td>
</tr>
<tr>
<td>Insurance, Interest &amp; Bad Debt</td>
<td>1,192</td>
<td>1,892</td>
<td>3,084</td>
</tr>
<tr>
<td>Contractual &amp; Special Services</td>
<td>59,966</td>
<td>40,806</td>
<td>100,772</td>
</tr>
<tr>
<td>Other Expenditures</td>
<td>(581)</td>
<td>1,842</td>
<td>1,261</td>
</tr>
<tr>
<td>Subgrants &amp; Subcontracts</td>
<td>189,166</td>
<td>189,166</td>
<td>0</td>
</tr>
<tr>
<td>Cost Sharing</td>
<td>991,200</td>
<td>991,200</td>
<td>1,425,059</td>
</tr>
<tr>
<td>Total Non-Personnel</td>
<td>747,594</td>
<td>1,345,966</td>
<td>2,093,560</td>
</tr>
<tr>
<td>GRAND TOTAL</td>
<td>3,261,545</td>
<td>3,648,421</td>
<td>6,909,966</td>
</tr>
</tbody>
</table>

### Revenue

<table>
<thead>
<tr>
<th></th>
<th>FY13-14 Actual</th>
<th>FY14-15 Proposed</th>
<th>FY15-16 Requested</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Appropr.</td>
<td>Total</td>
<td>Appropr.</td>
</tr>
<tr>
<td>Carryover State Appropriation</td>
<td>1,807,632</td>
<td>1,807,632</td>
<td>2,055,238</td>
</tr>
<tr>
<td>New Matching Funds</td>
<td>3,261,545</td>
<td>3,261,545</td>
<td>3,422,020</td>
</tr>
<tr>
<td>Carryover from Previous Matching Funds</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Total Revenue</td>
<td>3,261,545</td>
<td>5,703,659</td>
<td>8,965,204</td>
</tr>
</tbody>
</table>

Note: FY 13 Actual Appropriations expenditures and carryover were reported incorrectly due to $24,185 of expenses on R011024318 not included.
All qualified applicants will receive equal consideration for employment and admissions without regard to race, color, national origin, religion, sex, pregnancy, marital status, sexual orientation, gender identity, age, physical or mental disability, or covered veteran status.

Eligibility and other terms and conditions of employment benefits at The University of Tennessee are governed by laws and regulations of the State of Tennessee, and this non-discrimination statement is intended to be consistent with those laws and regulations.

In accordance with the requirements of Title VI of the Civil Rights Act of 1964, Title IX of the Education Amendments of 1972, Section 504 of the Rehabilitation Act of 1973, and the Americans with Disabilities Act of 1990, The University of Tennessee affirmatively states that it does not discriminate on the basis of race, sex, or disability in its education programs and activities, and this policy extends to employment by the University.

Inquiries and charges of violation of Title VI (race, color, national origin), Title IX (sex), Section 504 (disability), ADA (disability), Age Discrimination in Employment Act (age), sexual orientation, or veteran status should be directed to the Office of Equity and Diversity (OED), 1840 Melrose Avenue, Knoxville, TN 37996-3560, telephone (865) 974-2498 (V/TTY available) or 974-2440. Requests for accommodation of a disability should be directed to the ADA Coordinator at the Office of Equity and Diversity.

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