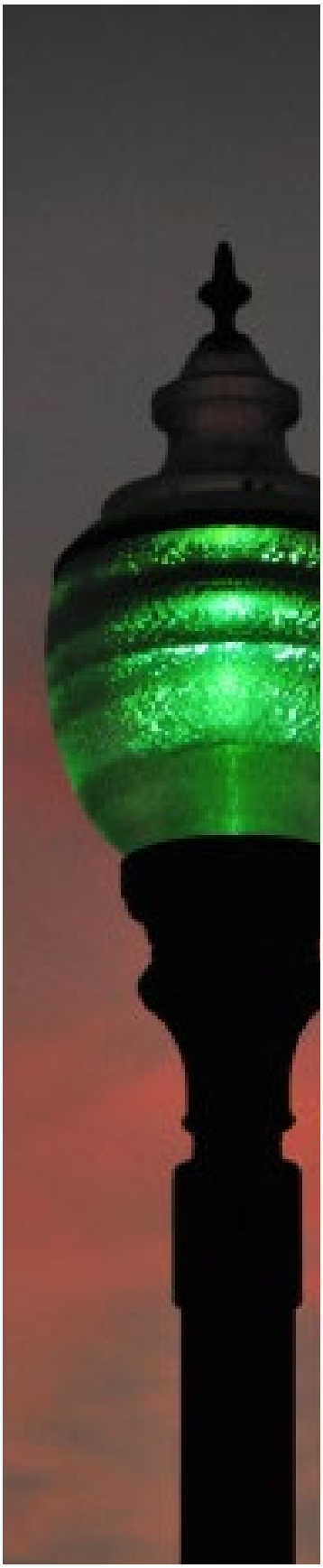


UT-ORNL Science Alliance

July 1, 2013–June 30, 2014

Annual Report

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.

Contents

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

Assistant Director	Lynne Parker
Business Manager	Betty Carmon
Accounting Specialist II	Missy Hodge

Science Alliance Span of Operation
July 1984–2014

Vice Chancellor for Research & Engagement

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

Dr. 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.

External Research Funds Awarded to UT-ORNL Distinguished Scientists in FY14

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.

Divisional Assoc. Editor in Condensed Matter Physics - Physical Review Letters.

David Joy

In conjuction 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.

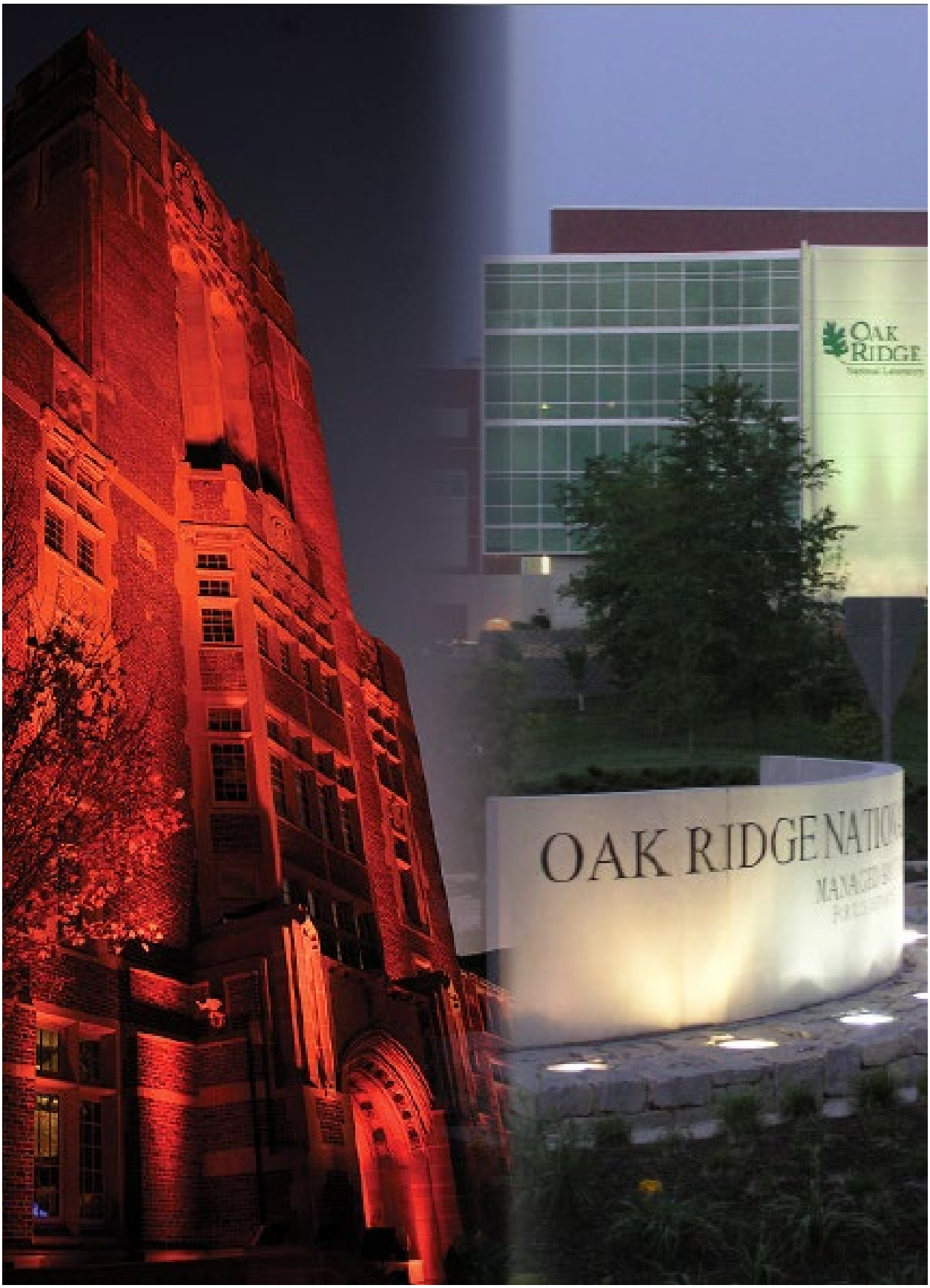
Recipient of Bill & Melinda Gates Foundation Grand Challenges Explorations Award.

Prin Inv	Project Name	Project Title	Start Date	End Date	Award Amount	FY 14 Expenditures
Dagotto	UT-B 4000099504	Theoretical Studies of Model Hamiltonians	09/29/2010	09/30/2013	173,315	20,285
Dagotto	NSF-DMR-1104386	Computational Studies of Model Hamiltonians for Pnicctides and Multiferroic Manganites	09/01/2011	08/31/2014	420,000	251,303
Egami	JINS Enrichment Fund	JINS Enrichment Fund	07/01/2005	12/31/2047	29,000	244
Egami	UT-B 4000119538	Physics of Metallic Glasses	01/01/2013	12/31/2014	356,884	236,293
Egami	UT-B 4000131427 Egami	Local Structure by Neutron Diffraction	07/01/2014	06/30/2015	180,000	-
Egami	DOE-DE-FG02-08ER46528-004	Neutron Scattering Research Network for EPSCOR States	09/01/2008	05/31/2015	1,114,600	629,447
Egami	DOE-DE-FG02-08ER46528	Neutron Scattering Research Network for Epscor States	09/01/2008	05/31/2014	1,980,000	-
Egami	DOE-DE-FG02-08ER46528	Neutron Scattering Research Network for Epscor States - Dept. Matching	09/01/2008	05/31/2015	-	105,733
Egami	UT-B 4000111177	Unilamellar Vesicles as Platforms for Understanding Biological Phenomena	01/09/2012	07/31/2013	73,804	2,965
Egami	DOE-FG02-08ER46528	Neutron Scattering Research Network for Epscor States	09/01/2008	05/31/2015	69,070	-
Egami	DOE-DE-FG02-08ER46528-Matching-Egami 10	Neutron Scattering Research Network for Epscor States	09/01/2008	05/31/2015	34,543	-
Egami	ARRA-Washington Univ WU-HT-10-51	ARRA: Construction of the Parts for MRI-R2 Project	04/01/2010	09/30/2013	146,039	4,047
Egami	ARRA-Washington Univ WU-HT-10-51	ARRA: Construction of the Parts for MRI-R2 Project	04/01/2010	09/30/2013	-	1,335
Egami	UT-B 4000126542 Egami	Dynamics of Biologically Relevant Model Membrane Systems	09/20/2013	08/31/2015	87,210	41,837
Guiochon	DOE-DE-SC0001014	Separation of Highly Complex Mixtures by Two-Dimension Liquid Chromatography	09/19/2011	05/31/2013	120,000	7,864
Guiochon	Waters Technologies Corp 2013 Guiochon	Research in supercritical fluid chromatography	01/01/2013	04/30/2014	61,000	60,965
Guiochon	NSF CHE-1108681	Fundamental Studies in Nonlinear Chromatography	06/01/2011	12/31/2014	175,000	-
Guiochon	NSF CHE-1108681	Fundamental Studies in Nonlinear Chromatography	09/19/2011	12/31/2014	350,000	164,378

External Funding – FY14

Prin Inv	Project Name	Project Title	Start Date	End Date	Award Amount	FY 14 Expenditures
Hatcher	NRC-HQ-11-G-04-0085 Hatcher	Two-Year Collaborative Research Project to Assess Large Earthquake Seismology in the ETSZ	09/26/2011	09/25/2015	454,706	88,548
Hatcher	USGS G13AC00089 Hatcher	Detailed Geologic Mapping of Quaternary French Broad River Terraces, Eastern Tennessee	05/01/2013	04/30/2014	8,217	6,745
Hatcher	USGSG13AC00089 C/S Hatcher	Detailed Geologic Mapping of Quaternary French Broad River Terraces, Eastern Tennessee	05/01/2013	07/31/2014	9,334	4,007
Hatcher	USDI-NPS P14AC00244-Hatcher	Geologic Mapping of the Lancing, Hebbertsburg, and Fo Creek 7.5 minute quadrangles, Wild and Scenic River	04/01/2014	03/31/2015	43,537	14,163
Joy	Electron Microscopy Facility	Unrestricted Research Support	04/11/1989	12/31/2047	-	-
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	29,073
Macek	DOE-DE-FG02-02ER15283-MACEK 12 49%	Theory of Atomic Collisions and Dynamics	03/01/2012	02/28/2015	376,000	128,776
Mays	Dow Chemical Co. - Jimmy Mays	Unrestricted Research Support	10/30/2002	12/31/2047	35,000	-
Mays	UT-B 4000076055	Plymer-Based Multicomponent Materials	11/20/2008	09/30/2013	161,386	3,154
Mays	NSF-DMR-0906893	Collaborative Research: Synthesis and Rheology of Strategically Designed Long-Chain-Branched Polymers	09/01/2009	08/31/2013	160,000	6,438
Mays	UT-B 4000105959	Fundamentals of Ionic Conductivity in Polymeric Materials for Energy Storage Applications: How to Decouple Ionic Motions from Segmental Dynamics	06/08/2011	08/31/2013	89,599	941
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	38,366	38,366
Mays	Eastman Chemical Co Synthesis Polyethyl Mays	Synthesis of Miktoarm Star Polymers	05/01/2013	04/30/2014	6,000	6,000

Prin Inv	Project Name	Project Title	Start Date	End Date	Award Amount	FY 14 Expenditures
Mays	Dow Chemical Co. Synthesis Polyethyl Mays	Synthesis of H Polyethylenes	02/01/2014	06/30/2014	20,000	18,281
Mays	Navy ONR N00014-10-1-0393	Nanofiller Reinforced Nonwoven Sandwiched Composites	01/17/2012	06/30/2014	48,372	1,645
Mays	UT-B 4000121786	UT-Synthesis of Organic Nanomembranes	04/01/2013	08/31/2013	17,000	2,548
Mays	Vanderbilt Univ Sub No. 2016-015735	Improved Carbon Nanotube Fibers through Crosslinking and Densification	01/01/2013	12/31/2014	247,500	169,472
Mays	Vanderbilt Univ Sub No. 2016-015735		01/01/2013	12/31/2014	49,813	72,933
Mays	NSF-IIP-1237787	PFI-BIC: Superelastomers: New Thermoplastic Elastomers Based on Multigraft Copolymers	09/01/2012	08/31/2015	493,258	259,186
Mays	Bill & Melinda Gates Fnd OPP1098281 Mays	Ultra-Sensory Condoms Based on New Superelastomer Technology	01/01/2013	04/30/2015	100,000	60,472
		Total External Funds			$7,840,526	$2,437,444
		Total Distinguished Scientist ORNL Match			$1,085,982	$992,948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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.

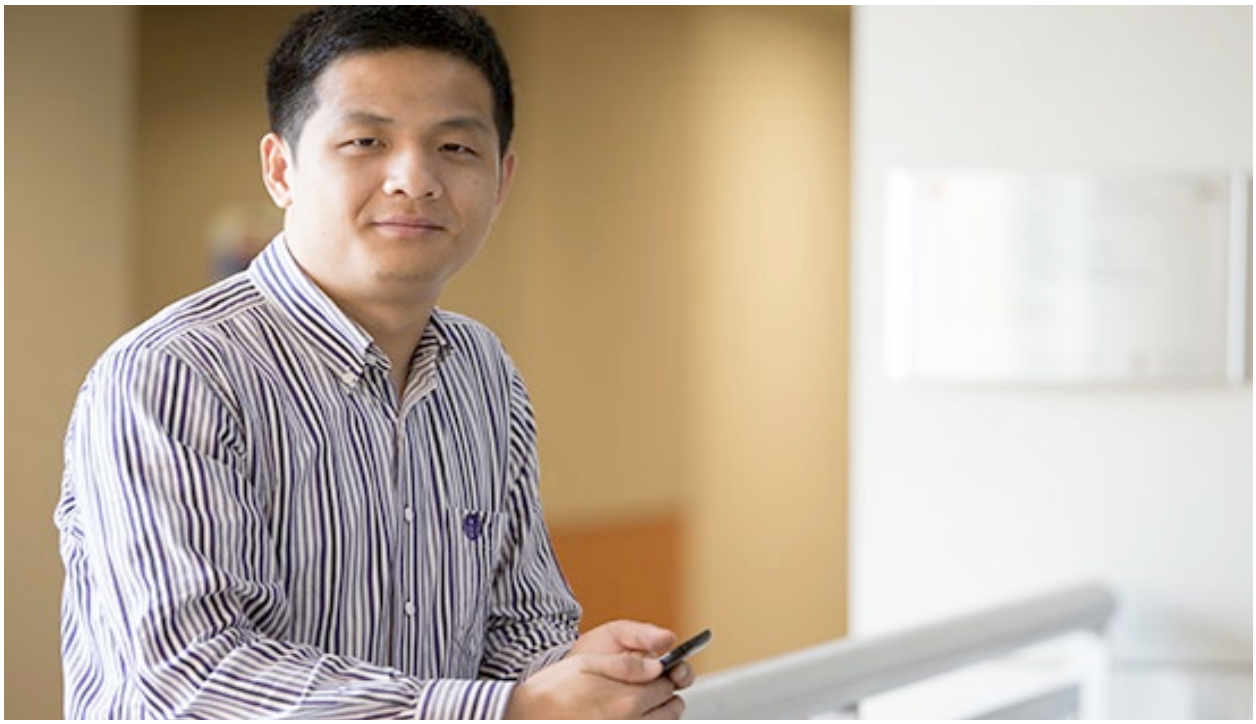
Often large and complex, life-sustaining molecules are composed of multiple stable units called domains—each with a distinct structure and function; each conserved in near identical form from specie to specie.

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.

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

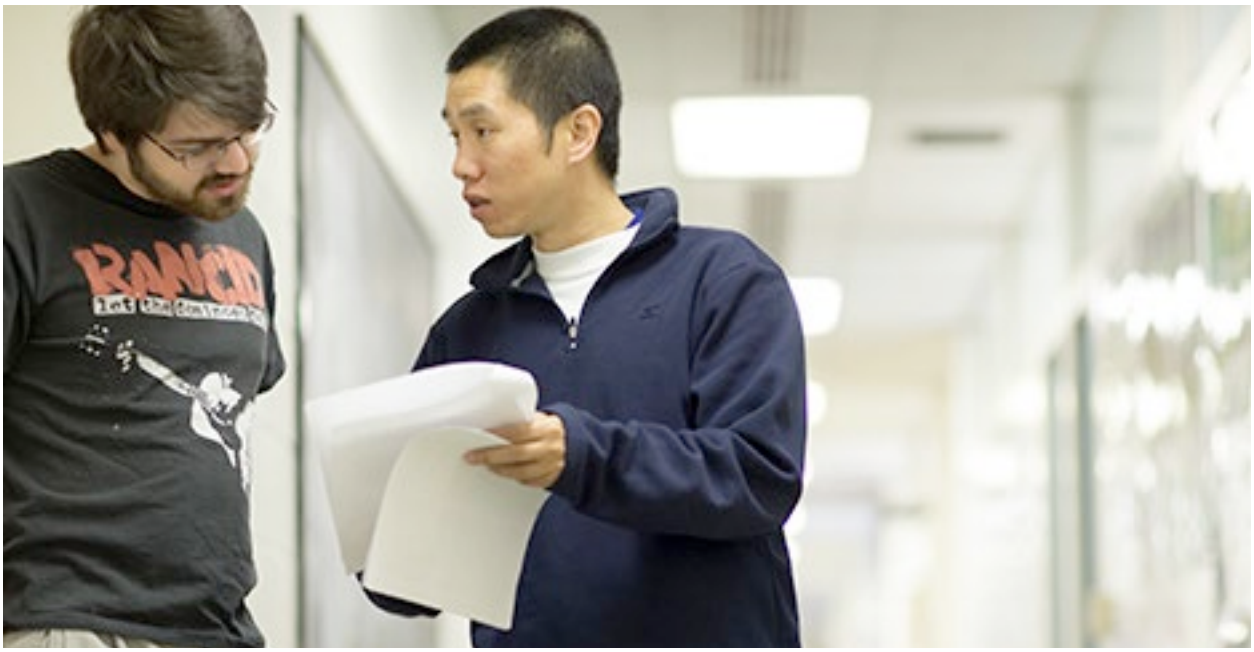
Cell membranes teach us about "how things work" in the natural world.

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 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

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.

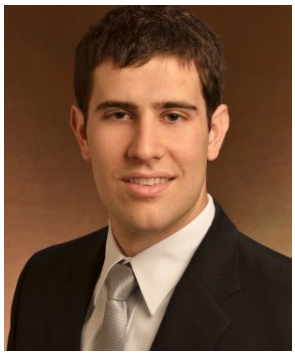
Our ability to understand the dynamic motions of proteins is what really counts when we peer into biological systems and observe how they respond to change. Increasingly complex studies of protein systems—as they change shapes to regulate and signal biological processes—hold enormous promise for advances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

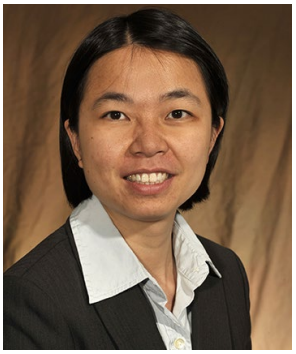
JDRD funding could improve the performance of hybrid electric vehicles.

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 Biocompatability 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.

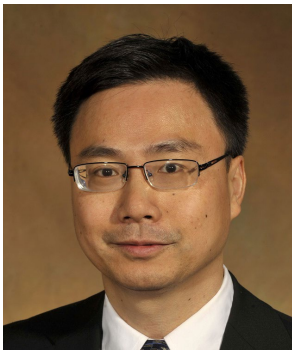
Nanocellulose, a type of nanomaterials of natural origin with great abundance and high renewability, is fueled by its excellent mechanical properties. Nanocellulose has recently made inroads into the biomedical field.

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

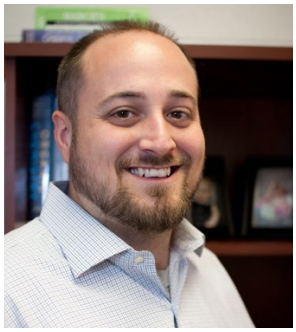
Dr. Mingzhou Jin hopes algorithm development will change the future for plug-in electric vehicles.

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 (CO_2) 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 CO_2 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 CO_2 separations.

Specifically, they have developed and thoroughly investigated a class of highly rigid yet highly porous polymers that contain CO_2-philic, or CO_2 loving functionalities. These polymers have demonstrated remarkable CO_2 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.

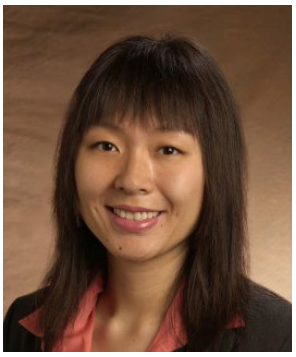
When the current and voltage across a MESFET is large, device self-heating leads to performance degradation. Diamond has a large band gap and the highest thermal conductivity of any semiconductor, so its application for high power devices show promise.

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.

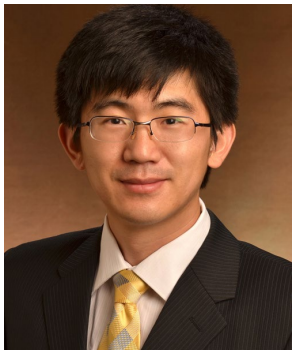
Sun's JDRD team is researching Multi-factor authentication based on user behavior.

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.

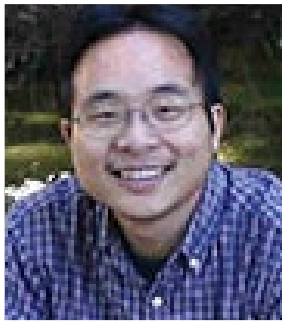
This research is an effort to build a strong representation of MGI-related research in advanced materials, which enhances not only the UT/ORNL relationship but also the preparedness of UT's research portfolio in MGI.

In particular, this project is going to examine the defect transport properties of a large number oxide supperlattice 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

ORNL 2014-G00877/asg

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.

Collaborative Cohort Program

Stephanie TerMaath

Assistant Professor, Civil and Environmental Engineering
Cohort Project:
Supercomputing for Multi-Disciplinary Optimization of Obstructed Ventricular Catheters

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

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Al-Hassanieh, K.A., Rincon, J., Dagotto, E., and Alvarez, G., "Wave-packet dynamics in the one-dimensional extended Hubbard model," *Phys. Rev. B* 88:045107 (2013).

Liang, S., Moreo, A., and Dagotto, E., "Nematic State of Pnictides Stabilized by Interplay between Spin, Orbital, and Lattice Degrees of Freedom" *Phys. Rev. Lett.* 111:047004 (2013).

Guo, H., Noh, J.H., Dong, S., Rack, P.D., Gai, Z., Xu, X., Dagotto, E., Shen, J., and Ward, T.Z., "Electrophoretic-like Gating Used To Control Metal-Insulator Transitions in Electronically Phase Separated Manganite Wires," *Nano Lett,* 13:3749-3754 (2013).

Lv, W., Moreo, A., and Dagotto, E., "B1g-like pairing states in two-leg ladder iron superconductors," *Phys. Rev. B* 88:094508 (2013).

Dong, S., and Dagotto, E., "Full control of magnetism in a manganite bilayer by ferroelectric polarization," *Phys. Rev. B* 88:140404(R) (2013).

Jiang, L., Choi, W.S., Jeen, H., Dong, S., Kim, Y., Han, M., Zhu, Y., Kalinin, S.V., Dagotto, E., Egami, T., and Lee, H.N., "Tunneling Electroresistance Induced by Interfacial Phase Transitions in Ultrathin Oxide Heterostructures," *Nano Lett.*, 13:5837.

Takashi Egami

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

Egami, T., Iwashita, T., and Dmowski, W., "Mechanical Properties of Metallic Glasses," *Metals*, 3:77 (2013).

Levashov, V.A., Morris, J.R., and Egami,, T., "The Origin of Viscosity as seen through Atomic Level Stress Correlation Function," *J. Chem. Phys.* 138:044507 (2013).

Zhang, C., Liu, M., Su, Regnault, L.P, Wang, M., Tan, G., BrÄuckel, T., Egami, T., and Dai, P., "Magnetic Anisotropy in Hole-doped Superconducting Ba0.67K0.33Fe2As2 Probed by Polarized Inelastic Neutron Scattering," *Phys. Rev. B*, 87:081101 (2013).

Nagase, T., Anada, S., Rack, P.D., Noh, J.H., Yasuda, H., Mori, H., and Egami, T., "MeV Electron Iirradiation-Induced Structural Change in the bcc Phase of Zr-Hf-Nb Alloy with an Approximately Equiatomic Ratio," *Intermetallics*, 38:70 (2013).

Tong, Y., Dmowski, W., Witczak, Z., Chuang, C.P., and Egami, T., "Residual Elastic Strain induced by Equal Channel Angular Pressing on Bulk Metallic Glasses," *Acta Mater.* 61:1204 (2013).

Guo, W., Dmowski, W., Rack, Ph., Liaw, P., and Egami, T., "Local Atomic Structure of a High-Entropy Alloy: An X-ray and Neutron Scattering Study" *Metall. Mater. Trans. A*, 44:1994 (2013).

Wu, B., Liu, Y., Li, X., Mamontov, Kolesnikov, A.I., Diallo, S.O., Do, C., Porcar, L., Hong, K., Smith, S.C., Liu, L., Smith, G.S., Egami, T., and Chen, W.R., "Charge-Dependent Dynamics of a Polyelectrolyte Dendrimer and Its Correlation with Invasive Water," *J. Amer. Chem. Soc.*, 135:5111 (2013).

Iwashita, T., Nicholson, D.M., and Egami, T., "Elementary Excitations and Crossover Phenomenon in Liquids" *Phys. Rev. Lett.*, 110:205504 (2013).

Tong, Y., Dmowski, W., Yokoyama, Y., Wang, G., Liaw, P.K., and Egami, T., "Recovering Compressive Plasticity of Bulk Metallic Glasses by High Temperature Creep" *Scripta Mater.*, 69:570 (2013).

Nicholson, D.M., Ojha, M., and Egami, T., "First Principles Local Stress in Crystalline and Amorphous Metals," *J. Phys.: Condens. Matt.*, 25:435505 (2013).

Tang, Z., Diao, H., Yang, T., Liu, J., Zhang, Y., Zuo, T., Gao, M.C., Lu, Z., Dahmen, K.A., Zhang, Y., Liaw, P.K., and Egami, T., "Aluminum Alloying Effects on Lattice Types, Microstructures, and Mechanical Behavior of High-Entropy Alloys Systems," *J. Metals,* 65:1848 (2013).

Zhang, C., Yu, R., Su, Y., Song, Y., Wang, M., Tan, G., Egami, T., Fernandez-Baca, J.A., Faulhaber, E., Si, Q., and Dai, P., "Measurement of a Double Neutron Spin Resonance and an Anisotripic Energy Gap for Underdoped Superconducting NaFe0.985Co0.015As Using Inelastic Neutron Scattering," *Phys. Rev. Lett.*, 111:207002 (2013).

Jiang, L., Coi, W.S., Jeen, H., Dong, S., Kim, Y., Kalinin, S.V., Dagotto, E., Egami, T., and Lee, H.N., "Tunneling Electroresistance Induced by Interfacial Phase Transitions in Ulterthin Oxide Heterostructures," *Nano-Letters*, 13:5837 (2013).

Georges Guichon

UT Department of Chemistry

Stevenson, P.G., Gao, H., Gritti, F., and Guiochon, G., "Optimization of the boundary locations for calculations of the second peak moment." *J. Separat. Sci.*, 36:279–287 (2013).

Gritti, F., and Guiochon, G., "Speed-resolution properties of columns packed with new 4.6 µm Kinetex-C18 core-shell particles," *J. Chromatogr. A*, 1280:35–50 (2013).

Gritti, F., and Guiochon, G., "Adsorption behaviors of neutral and ionizable compounds on hybrid stationary phases in the absence (BEH-C18) and the presence (CSH-C18) of immobile surface charges," *J. Chromatogr. A*, 1282:47–57 (2013).

Gritti, F., and Guiochon, G., "Study of the adsorption process of an ionic surfactant onto a new RPLC-IEC mixed-mode stationary phase." *J. Chromatogr. A*, 1282:58–71 (2013).

Gritti, F., and Guiochon, G., "Effect of the pH and the ionic strength on overloaded band profiles of weak bases onto neutral and charged surface hybrid stationary phases in RPLC," *J. Chromatogr. A*, 1282:113–126 (2013).

Tarafder, A., Guiochon, G., "Accurate measurements of experimental parameters in supercritical fluid chromatography. I. Extent of variations of the mass and volumetric flow rates," *J. Chromatogr. A*, 1285:148–158 (2013).

Gritti, F., and Guiochon, G., "Perspectives on the evolution of the column efficiency in liquid chromatography," *Anal. Chem.*, 85:3017–3035 (2013).

Gritti, F., Guiochon, G., "Gradient chromatography under constant frictional heat. Realization and application," *J. Chromatogr. A*, 1289:1–12 (2013).

Gritti, F., Tarafder, A., Guiochon, G., "Interpretation of dynamic frontal analysis data in solid/supercritical fluid adsorption systems. I- Theory," *J. Chromatogr. A*, 1290:73–81.

Vajda, P., Felinger, A., Guiochon, G., "Evaluation of surface excess isotherms in liquid chromatography," *J. Chromatogr. A*, 1291:41–97 (2013).

Gritti, F., Guiochon, G., "Realization and potential advantages of gradient separations performed under steady state temperature regime," *J. Chromatogr. A*, 1291:104–113 (2013).

Kaczmarski, K., Poe, D.P., Tarafder, A., Guiochon, G., "Efficiency of Supercritical Fluid Chromatography Columns in Different Thermal Environments," *J. Chromatogr. A*, 1291:155–173 (2013).

Gao, H., Gritti, F., and Guiochon, G., "Investigations on the calculation of the third moments of elution peaks. II- Consideration about external mass transfer coefficient," *J. Chromatogr. A*, 1294:41–49 (2013).

Gritti, F., and Guiochon, G., "Limit of the speed-resolution properties in adiabatic supercritical fluid chromatography," *J. Chromatogr. A*, 1295:114–127 (2013).

Gritti, F., Guiochon, G., "Effect of parallel segmented flow chromatography on the height equivalent to a theoretical plate. I- Performance of 4.6 x 30 mm columns packed with 3.0 µm Hypersil-C18 fully porous particles," *J. Chromatogr. A*, 1297:64–76 (2013).

Gritti, F., and Guiochon, G., "Comparison between the intra-particle diffusivity in the Hydrophobic Interactions Chromatography and RPLC modes. Impact on the column efficiency," *J. Chromatogr. A*, 1297:85–95 (2013).

Gritti, F., and Guiochon, G., "Mass transfer mechanism in Hydrophobic Interactions Chromatography," *J. Chromatogr. A*, 1302:55–64 (2013).

Gritti, F., and Guiochon, G., "The van Deemter equation. Assumptions, limits, and adjustment to modern high performance Liquid Chromatography," *J. Chromatogr. A*, 1302:1–13 (2013).

Gritti, F., and Guiochon, G., "The van Deemter equation. Assumptions, limits, and adjustment to modern High Performance Liquid Chromatography," *Journal of Chromatography A*, 1302:1–13 (2013).

Vajda, P., Guiochon, G., "Modifier adsorption in supercritical fluid chromatography onto silica surface," *Journal of Chromatography A*, 1305:293–299 (2013).

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

SFC column I-Linear conditions," *Journal of Chromatography A,* 1306:89–96 (2013).

Vajda, P., Guiochon, G., "Surface excess isotherms of organic solvent mixtures in a system made of liquid carbon dioxide and a silicagel surface," *Journal of Chromatography A*, 1308:139–143 (2013).

Vajda, P., and Guiochon, G., "The effect of the back pressure and the temperature on the finite layer thickness of the adsorbed phase layer in supercritical fluid chromatography," *Journal of Chromatography A*, 1309:41–47 (2013).

Vajda, P., and Guiochon, G., "Determination of the column hold-up volume in supercritical fluid chromatography using nitrous-oxide," *Journal of Chromatography A*, 1309:96-100 (2013).

Stankovich, J.J., Gritti, F., Stevenson, P.G, and Guiochon, G., "The Impact of Column Connections on Band Broadening in Very High Pressure Liquid Chromatography," *Journal of Separation Science*, 36:2709–2717 (2013).

Gritti, F., Guiochon, G., "Analytical solution of the ideal model of chromatography for a bi-Langmuir adsorption isotherm," *Analytical Chemistry*. 85:8552–8558 (2013).

Gritti, F., and Guiochon, G., "Effect of parallel segmented flow chromatography on the height equivalent to a theoretical plate. II- Performances of 4.6x30 mm columns packed with 2.6 μm Accucore-C18 superficially porous particles," *Journal of Chromatography A*, 1314:54–63 (2013).

Gritti, F., and Guiochon, G., "Effect of methanol concentration on the speed-resolution properties in adiabatic supercritical fluid chromatography," *Journal of Chromatography A*, 1314:255–265 (2013).

Kamarei, F., Tarafder, A., Gritti, F., Guiochon, G., "Determination of the adsorption isotherm of the Naproxen enantiomers on (S,S)-Whelk-O1 in supercritical fluid chromatography," *Journal of Chromatography A*, 1314:276–287 (2013).

Gritti, F., Neue, U., Iraneta, P., and Guiochon, G., "Adsorption onto charged surface mesopores. I-Theory," *Journal of Chromatography A*, 1318:72–783 (2013).

Stankovich, J.J., Gritti, F., Beaver, L.A., Stevenson, P.G., and Guiochon, G., "Fast Gradient Separation by Very High Pressure Liquid Chromatography: Reproducibility of Analytical Data and Influence of Delay between Successive Runs," *Journal of Chromatography A*, 1318:122–133 (2013).

Hlushkou, D., Gritti, F., Daneyko, A., Guiochon, G., and Tallarek, U., "How Microscopic Characteristics of the Adsorption Kinetics Impact Macroscale Transport in Chromatographic Beds," *The Journal of Physical Chemistry C*, 117:22974–22985 (2013).

Robert Hatcher

UT Department of Earth and Planetary Science

Huebner, M. T., and Hatcher, R. D., "Polyphase reactivation history of the Towaliga fault, central Georgia: Implications regarding the amalgamation and breakup of Pangea," *Journal of Geology*, 121:75-90 (2013).

Steltenpohl, M. G., Horton, J.W., Jr., Hatcher, R.D., Jr., Zietz, I., Daniels, D.L., and Higgins, M.W., "Upper crustal structure of Alabama from regional magnetic and gravity data: Using geology to interpret geophysics, and vice versa," *Geological Society of America Geosphere*, 9:1-21 (2013).

David C. Joy

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

Joy, D.C. and Michael, J., "Modeling Ion-Solid Interactions for Imaging Applications," *Materials Research Society Bulletin, May* 123-139 (2013).

Joy, D.C., "Helium Ion Microscopy – Principles and Applications," published in the "Springer Briefs in Materials" series by Springer-Verlag; New York, December 2013.

He, Q., Surawerra S., Joy, D.C., Keffer, D.J., "Structure and Properties of the Interfacial Bonding Layer in Proton Exchange Membrane Fuel Cells," *J.Phys.Chem C*, 1021-1029 (2013).

He, Q., Chen, J., Keffer, D.J., Joy, D.C., "Electron Beam Induced Radiation Damage in the Catalyst Layer of a Proton Exchange Membrane Fuel Cell", *SCANNING*, 1002-5 (2013).

He, Q., Joy, D.C., Keffer, D.J., "Impact of Oxidation on Nanoparticle Adhesion to Carbon

Substrates," *Royal Society of Chemistry Advances 3*, 15792-15804 (2013).

He, Q., Joy, D.C., Keffer D.J., "Nanoparticle adhesion in proton exchange membrane fuel cell electrodes," *J.Power Sources* 241:634-646 (2013).

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Wang, Q., Keffer, D.J., Deng, S., and Mays, J., J. Phys. Chem. C, "Structure and Diffusion in Cross-linked and Sulfonated Poly (1, 3-cyclohexadiene)Polyethylene Glycol-based Proton Exchange Membranes," *J. Phys. Chem C*. 54 117:4901-4912 (2013).

Hosoda, T., Gido, S., Mays, J., Huang, T., Park, C.R., and Yamada, T., "Effects of Solvents and Thermal Annealing on the Morphology Development of a Novel Block Copolymer Ionomer; a Case of Study Sulfonated Polystyrene-b-Fluorinated Polyisoprene," *Journal of Polymer Engineering,* 33(1):49-59 (2013).

Kumar, R., Sides, S.W., Goswami, M., Sumpter, B.G., Hong, K., Wu, X., Russell, T.P., Gido, S.P., Rangou, S., Misichronis, K., Avgeropoulos, A., Tsoukatos, T., Hadjichristidis, N., Beyer, F.L., and Mays, J.W., "Morphologies of ABC tri-block terpolymer melts containing poly(cyclohexadiene) : effects of conformational asymmetry," *Langmuir*, 29:1995 (2013).

Misichronis, K., Rangou, S., Ashcraft, E., Kumar, R., Sumpter, B., Dadmun, M., Mays, J.W., Zafeiropoulos, N., and Apostolos, A., "Synthesis, Characterization, and Theoretical Morphology Predictions of Poly(cyclohexadiene) Containing Triblock Copolymers," *Polymer*, 54:1480 (2013).

Wang, Q., Keffer, D. J., Deng, S., and Mays, J.W., "Structure and Proton Transport in Proton Exchange Membranes Based on Crosslinked Sulfonated Poly(1,3-cyclohexadiene) with Varying Local Acid Environment," *Polymer*, 54:2299-2307 (2013).

Ruppel, M., Pester, C., Schoberth, H., Schmidt, K., Urban, V., Mays, J.W., Böker, A., "Electric-Field Induced Selective Disordering in Lamellar Block Copolymers," *ACS Nano*, 7:3854 - 3867 (2013).

Misichronis, K., Rangou, S., Ashcraft, E., Kumar, R., Sumpter, B., Dadmun, M., Mays, J.W., Zafeiropoulos, N., and Apostolos, A., "Synthesis, Characterization, and Theoretical Morphology Predictions of Poly(cyclohexadiene) Containing Triblock Copolymers" *Polymer*, 54:1480-1489 (2013).

Dyer, C., Driva, P., Sides, S.W., Sumpter, B.G., Mays, J.W., Chen, J., Kumar, R., Goswami, M., and Dadmun, M., "Effect of Macromolecular Architecture on the Morphology of Polystyrene-Polyisoprene Block Copolymers," *Macromolecules*, 46:2023-2031 (2013).

Tsiamantas, C., Psarros, K., Mays, J.W., and Pitsikalis, M., "Micellization Behavior of Model Asymmetric Miktoarm Star Copolymers of the AA'B Type, where A is Polyisoprene, PI, and B is Polystyrene" *Polymer Journal*, 45:1216-1223 (2013).

Zhu, J., Zhang, S., Zhang, K., Wang, X., Mays, J.W., Wooley, K.L., Pochan, D.J., "Disk-Cylinder and Disk-Sphere Nanoparticles via a Block Copolymer Blend Solution Construction" *Nature Communications*, 4, article 2297 (2013).

Chen, J., Alonzo, J., Yu, X., Hong, K., Messman, J.M., Ivanov, I., Lavrik, N.V., Banerjee, M., Rathore, R., Sun, Z., Li, D., Mays, J.W., and Kilbey, S.M., Mater, J., "Grafting-Density Effects, Optoelectrical Properties and Nano-Patterning of Poly(para-Phenylene) Brushes" *Chem. A*, 1:13426-13432 (2013).

Ding, W., Lin, J., Yao, K., Mays, J.W., Ramanathan, M., and Hong, K., "Building Triangular Nanoprisms from the Bottom-up: A Polyelectrolyte Micellar Approach" *J. Mater. Chem. B*, 1:4212-4216 (2013).

Hua, F., Yuan, W., Britt, P.F., Mays, J.W., Hong, K., "Temperature-Induced Phase-Transitions of Methoxyoligo(oxyethylene) styrene-based Block Copolymers in Aqueous Solution," *Soft Matter*, 9:8897-8903 (2013).

Joint Directed Research and Development Publications

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UT Department of Civil and Environmental Engineering

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 Enginering. American Society of Civil Engineers (ASCE), 139:715-723 (2013).

Santos-Villalobos, H., Bingham, P., Gregor, J., "Iterative reconstruction of coded source neutron radiographs," *IEEE Transactions on Nuclear Science*, 60:1624-1631 (2013).

Santos-Villalobos, H., Bingham, P., Gregor, J., "Neutron imaging with coded sources: New challenges and the implementation of SIRT," *SPIE Electronic Imaging*, San Jose, Vol. 8657 (2013).

Toops, T., Bilheux, H., Voisin, S., Gregor, J., Walker, L., Strzelec, A., Finney, C., Pihl, J., Schillinger, B., and Schulz, M., "Neutron tomography of particulate filters: A non-destructive investigation tool for applied and industrial research," *Nuclear Instruments and Methods in Physics Research Section A* 729:581-588, (2013).

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UT Deparmtent of Chemistry

Murdock, C.R., Lu, Z.; Jenkins, D.M., "Effects of Solvation on the Framework of a Breathing Copper MOF Employing a Semirigid Linker. *Inorg. Chem.* 52:2182-2187 (2013).

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Ma, J., O. Delaire, A. F. May, C. E. Carlton, M. A. McGuire, L. H. VanBebber, D. L. Abernathy, G. Ehlers, Tao Hong, A. Huq, Wei Tian, V. M. Keppens, Y. Shao-Horn & B. C. Sales, "Glass-like phonon scattering from a spontaneous nanostructure in AgSbTe2," *Nature Nanotechnology 8*, 445–451 (2013).

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UT Department of Earth and Planetary Sciences

Cheng, C.-L., M. Gragg, E. Perfect, M. White, P. Lemiszki, and L.D. McKay. 2013. Sensitivity of injection costs to input petrophysical parameters in numerical geologic carbon sequestration models, *International Journal of Greenhouse Gas Control* 18:277-284 (2013).

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