ICTAS Connection

The newsletter of the Institute for Critical Technology and Applied Science at Virginia Tech

www.ictas.vt.edu

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SWIM suits up in pursuit of national designation

Ann Craig | Connection Editor | 540-231-2059 | annc@vt.edu

Water research is recognized as a core strength for Virginia Tech. "We have more than 100 expert faculty researchers already active in water research, including a National Academy of Engineering Fellow and a MacArthur Fellow," says Roop Mahajan, Director of the Institute for Critical Technology and Applied Science. "Top notch faculty members are well-poised to collaborate toward advancing the state of the art in water infrastructure, standards and measurement systems," adds Thomas Campbell, Associate Director for Special Projects at ICTAS.

In recognition of the national need and Virginia Tech's strengths in infrastructure management, ICTAS established a center of excellence in sustainable water infrastructure management (ICE SWIM). This center is co-directed by professors Marc Edwards and Sunil Sinha. Center research in sustainable water technologies is dedicated to the creation of future water solutions for our nation's current and future water needs, offering solutions as water sources worldwide are shrinking within growing populations and expanding agricultural activity. Water research is focused upon improving water infrastructure and distribution, water remediation, water conservation, and creating new and improved technologies for the effective treatment and desalination of waters for the creation of new water for our world. The faculty members participating in SWIM have achieved notable success in securing significant research funding support. Additionally, ICTAS has invested close to $900,000 in support of the center plus 5,122 sq. ft. of laboratory space.

Recently both SWIM and ICTAS have engaged in discussions with the Environmental Protection Agency (EPA) directed toward the possibility of designation as a national center. ICTAS hosted Dr. Steve Allbee, EPA Project Director of the Gap Analysis, as part of the ICTAS spring seminar series 2009. During his visit, Dr. Allbee expressed interest in the university's technical strengths and in the institutional support of interdisciplinary research provided through ICTAS. Subsequently, Sinha initiated follow-on discussions with EPA program managers. These discussions led to hosting of a two-day visit by EPA program managers on September 28-29, offering an opportunity for showcasing our research strengths and committed institutional support. "The potential represented by the presence of a national laboratory on the Virginia Tech campus and the related ability to exchange researchers among laboratories underscores heretofore untapped opportunity for expanded research and education," says Mahajan "as well as the ability to more effectively address the needs of the Nation for sustainable water management and measurement systems."

The current research program in water research at Virginia Tech is quite comprehensive, including highlights such as a national pipe database for analysis, data mining, modeling and performance prediction; advanced sensors for condition assessment and system rehabilitation QA/QC; a laboratory facility for condition assessment and system rehabilitation research; a controlled field test facility for condition assessment and system rehabilitation research; a certificate program in infrastructure management; and, an advanced asset management training program.

INSIDE

Virginia Tech
Invent the Future®

Charting a course for the future

Dr. Robert Walters | Vice President for Research
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The research mission of the university plays a critical role in the development of faculty, the education of our undergraduate and graduate students, in advancing discipline-based knowledge and in improving our quality of life. At Virginia Tech, interdisciplinary research has also expanded significantly, as our faculty explore complex systems positioned at the frontiers of traditional disciplines.

The past year has witnessed significant growth in both the quantity and interdisciplinary nature of research at Virginia Tech. During the past year, VT researchers have submitted proposals totaling more than $1.2 billion, and research expenditures have grown by more than 5% in a challenging economic environment. A growing percentage of this research is devoted to large, collaborative projects which engage engineers, scientists, business, and policy experts in interdisciplinary teams.

In March, 2009, ICTAS personnel transitioned from their temporary offices in the Corporate Research Center to a dedicated facility in the heart of the Virginia Tech campus. The new "ICTAS headquarters," which houses both ICTAS and the School of Biomedical and Engineering Sciences, provides a much needed locus for the Institute's collaborative work. This facility provides the shared laboratory and meeting space which will allow the spirit of collaboration to take root and flourish, while inculcating the ICTAS values of integrity, forward thinking, spirit of openness, and service in our next generation of researchers.

In July, ICTAS achieved another milestone, as more than a year of discussions with the Naval Surface Warfare Center (NSWC) in Dahlgren, Virginia, regarding shared technical and workforce development interests culminated in an agreement which holds significant promise for collaboration in a wide range of disciplines. This agreement renews VT's longstanding relationship with NSWC through a five-year, $7.5 million indefinite delivery/indefinite quantity contract and a Cooperative Research and Development Agreement (CRADA). This agreement is designed not only to benefit VT researchers, but also to enhance the continuing collaboration between VT faculty and undergraduate and graduate student researchers and NSWC's practicing engineers.

The innovation that ICTAS brings to the research enterprise also positions the university for new and exciting approaches that engage undergraduate students in research. Whether through summer or academic-year research, problem-based, or research-led learning, ICTAS research provides a strong platform for students to become engaged in collaborative, interdisciplinary research in a variety of emerging areas of critical importance. Through early engagement, we seek to encourage a larger percentage of our undergraduate students to pursue advanced studies in their field. Programs such as the ICTAS Doctoral Scholars program provide critical investment in the intellectual talent of our students, and a pathway for engagement in cutting-edge research.

ICTAS is poised to play a critical role in the exploration of the most challenging issues of our times, including sustainable energy, renewable materials, sustainable water, cognition and communication, nanoscale science and engineering, and the nano-bio interface. Addressing these global issues will require a new approach, from advancing the frontiers of knowledge in current disciplines, to the creation and fostering of new disciplines. Through both its research and workforce development foci, ICTAS is well-positioned to achieve its mission of achieving global prominence in "transformative, sustainable technologies geared to societal needs."

Growing in spirals

Roop Mahajan | ICTAS Director
rmahajan@vt.edu

After experiencing the inevitable moving-in hiccups, we feel more at home and settled in our new headquarters on the main campus. The pace of laboratory occupancy and research activity has picked up and the building is humming with intellectual excitement. Our students and faculty appear to enjoy the laboratory and office space -inviting and rich in the promise of large collaborative research. The building is proving to be an asset in the implementation of our philosophy of "Spiral Research" briefly described below.

An educational psychologist, Jerome Bruner proposed the spiral curriculum concept in his classic text *The Process of Education**. He advocated that a curriculum should revisit its basic ideas repeatedly as it develops, building upon them until the student has grasped the full formal apparatus associated with these concepts. We have adapted this concept to our work with a belief that by strategically revisiting our investments over a period of time, we can grow our interdisciplinary research not in a straight line but in an upward spiral instead. This is depicted pictorially in Figure 1.

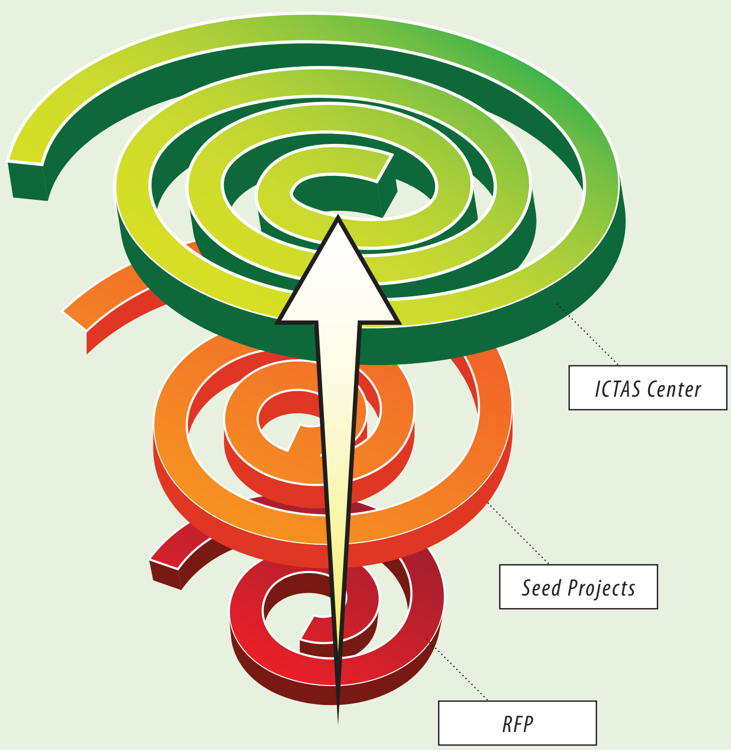
The first step in our research growth strategy is to provide seed monies through our yearly RFP (Request for Proposal) in which proposals are sought for investment and growth in the selected areas of interdisciplinary research aligned with our mission. The research conducted with the seed monies provides the preliminary data/proof of hypothesis and constitutes the first arm of the spiral.

Building on the preliminary data/research, the faculty are generally able to secure funds from external agencies (NIH, NSF etc), allowing them to expand their research to the next arm of the spiral: larger in scope and richer in content than the base arm. This process plays itself in one or more of our seed projects.

At this point in the upward spiral journey, ICTAS steps in to assess the possibility of bringing these faculty together under the umbrella of an ICTAS center, typically comprising of an interdisciplinary roster of twelve or more faculty members engaged in a multi-faceted research thrust with a significant potential for scholarship and large external funds. To ensure the sustainable growth of these centers, ICTAS commits an investment on the order of $75,000/year, on an on-going basis, with the expectation that the center will become eminent in its field and expand its research expenditures by a factor of two in five years. Our recently constituted centers- ICTAS Center for the Physics and Engineering of the Cell, ICTAS Center of Excellence in Sustainable Water Infrastructure (ICE SWIM) and ICTAS Center for Bio-Imaging are examples of the execution of this philosophy.

We are genuinely proud of the accomplishments of our faculty and students and share their excitement of discovery and learning. As we spiral upward in enhancing the research capacity and reputation of Virginia Tech in cutting-edge interdisciplinary research, we invite you to join us in this upward momentum.

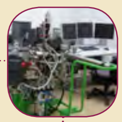
Figure 1.



*Bruner, J., *The Process of Education*. Cambridge, MA: Harvard University Press, 1960.

ICTAS
(Headquarters location on campus at Stanger Street)

The building is fully operational and is currently 90% occupied. While some laboratories are still being set up, research is well under way in most laboratories.



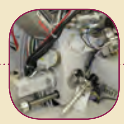
ICTAS – CRC
(Virginia Tech Corporate Research Center location)

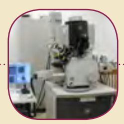
The Nanoscale Characterization and Fabrication Laboratory (NCFL), now in the second year of operation, is continuing to discover and support ways to grow business.

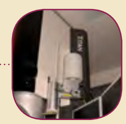
Research activity includes submission of seven proposals originated by NCFL scientists for extramural funding support and utilization of NCFL equipment and/or resources is incorporated in other proposals totaling $19 million. Additionally, NCFL has awarded mini-grants in support of proposal development, classes, start-up packages and cost sharing across the university.

In the learning domain, a graduate course in Scanning Transmission Electron Microscopy was offered during fall semesters 2008 and 2009 and an undergraduate course in nanotechnology is slated for spring 2010.

Several short courses have been delivered to the commercial community. This sector currently provides approximately 40% of the revenue supporting the NCFL.







ICTAS-LSC
(Life Sciences Corridor campus location)

Construction began in April and is well underway. The majority of the site work is complete and concrete pours of columns is underway. Construction completion is slated for early 2011.

This facility will be one of the first university facilities to be LEED certified. Skanska USA serves as the construction manager and design is by the Smith Group.

ICTAS-NCR
(National Capital Region Ballston location)

ICTAS will be expanding into the National Capital Region facility in the Ballston, Virginia area. The seven-floor, 144,000 square foot building, designed by Cooper Carry to meet the Silver U. S. Green Building Council's LEED™ Building Rating Systems, will be located on the 800-900 block of North Glebe Road. ICTAS is committed to approximately 6,000 square feet in this facility. The anticipated construction completion date is 2011.

ICTAS *Fall Seminar Series*

Friday, September 25, 2:30 - 4 pm, ICTAS, Room 310

Recent Investigations of Liquid Cooled Small-Scale Heat Sinks for High Flux Heat Removal: A Critical Summary of Experimental Data and Modeling Approaches

*with **Alfonso Ortega,** James R. Birle Professor of Energy Technology, Villanova University*

Tuesday, September 29, 4:30 - 5:30 pm, ICTAS, Room 310

Aging Water Infrastructure Research Program at US EPA - Addressing the Challenge through Innovation

*with **Daniel J. Murray,** Jr., Senior Environmental Engineer, U.S. Environmental Protection Agency*

Friday, October 30, 2009, 1:30 - 3:00 pm, ICTAS, Room 310

The Department of Energy's Fuel Cell Technologies Program

*with **Nancy Garland,** Program Manager, U.S. Department of Energy*

Thursday, November 5, 2009, 2:30 - 4:00 pm, ICTAS, Room 310

Low-Frequency Geometries for MEMS Vibrational Energy Harvesting

*with **M. Amin Karami,** ICTAS Doctoral Scholar*

Thursday, November 12, 3:00 - 4:30 pm, ICTAS, Room 310

Consumer Safety in a Rapidly Changing World: Security, Identity and Anti-Counterfeiting

*with **Steven Simske,** Director, Security Printing and Imaging, Hewlett-Packard Labs*

Friday, November 13, 2:00 - 4:30 pm, ICTAS, Room 310

Foundations for Future Physical Unclonable Functions

*with **Leyla Nazhandali** (ECE), **Patrick Schaumont** (ECE), and **Inyoung Kim** (STAT)*

Thursday, December 11, 2:30 - 4 pm, ICTAS, Room 310

Beyond Silos: Integrating Interdisciplinary Research and Education in the Academe

*with **Roop Mahajan,** ICTAS Director and James S. Tucker Professor of Engineering*

The ICTAS Seminar Series was launched in 2006 in concert with the arrival of the first permanent ICTAS Director, Roop Mahajan. The seminars aim to provide a forum for intellectual stimulation and exchange on a variety of topics.

At least one seminar per month is planned during the academic year period (September through April). Seminars are held in room 310 of the ICTAS headquarters building on Stanger Street on the main campus of Virginia Tech. Admission is free and light refreshments are available. Speaker nominations are welcomed and may be submitted to Ann Craig at 231-2059 or email: annc@vt.edu.

Cyber-engineering functional nanoparticles for targeted drug delivery

Gandour

Esker

Richard Gandour and Alan Esker | Targeted Delivery of Nanomedicine

Engineering versatile nanoparticles as drug delivery vehicles that enable simultaneous delivery of several agents is a key challenge in nanomedicine. The ability to simultaneously deliver therapeutic and neutriceutic agents to control infectious diseases, while reducing the emergence of resistant pathogens, with a simple formulation that ensures a uniform distribution of all agents is unattainable with current delivery systems. Frequently, the physicochemical properties of such a diverse combination of agents needed to effect this control differ widely. Some agents may be hydrophobic (insoluble in water) and others may be hydrophilic (soluble in water). Liposomes, which encapsulate an aqueous solution inside a hydrophobic bilayer membrane, can deliver both hydrophobic and hydrophilic agents. While liposomes have been studied for drug delivery vehicles since the 1970s, their efficacy has been limited by stability issues.

Three years ago, Alan Esker and Rich Gandour from the Department of Chemistry decided to tackle this limitation. They thought that liposomes would gain significant stability and functional capacity by having a solid core, tethered to the bilayer by strong linkers. Nevertheless, designing and constructing such complex nanoparticles posed an additional challenge. They contacted Amadeu Sum (then, a Virginia Tech faculty member in Chemical Engineering who subsequently moved to Colorado School of Mines in 2008) to collaborate on simulating the construction of such a nanoparticle. This collaboration led to a seed grant from ICTAS in 2007 to initiate the project. The preliminary data gathered during the subsequent 18 months uncovered further challenges that required additional help in modeling and design. The opportunity came in the form of the NSF Cyber-enabled Discovery and Innovation program. Sum recruited Roland Faller, Joe and Essie Smith Endowed Associate Professor of Chemical Engineering at the University of California Davis, and Markus Deserno, Associate Professor of Physics at Carnegie-Mellon University, to the project. Professor Faller led the proposal with Sum and Deserno rounding out the theoretical portion of the team, while Esker and Gandour covered the experimental side. NSF funded the resulting proposal for four years at more than $1.5M.

The funded project employs a multidisciplinary, multi-site strategy (Figure 1) that transforms conventional laboratory-centered synthesis into cyber-based nano-design. Its three key components are: (1) a multiscale modeling hierarchy (see **Table 1**) bridging the divide between molecules and physical meso-structure; (2) novel design- and parameter-optimization algorithms that exploit autonomous data exchange and learning over a distributed grid; and (3) a feedback system, in which simulations guide syntheses of improved nanoconstructs, while in vitro characterization validates and improves their corresponding in silico representations. Establishing a virtual organization that links four institutions (UC Davis, Colorado School of Mines, Carnegie Mellon, and Virginia Tech) maximally exploits joint expertise across a broad spectrum of disciplines and enables partnerships with others at these institutions. This cyber-infrastructure also enables a transformative approach to the rational computer-enabled design of functional nanoconstructs.

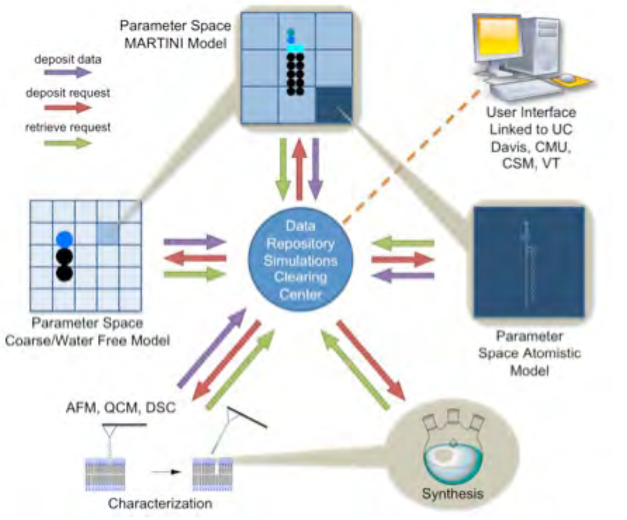


Figure 1. Illustration of the cyber-infrastructure proposed to enable the interplay among different scales and knowledge.

The cyber framework under development (**Figure 1**) will serve as a model for developing a real-time, virtual network that links computational and experimental science. For instance, this research will demonstrate how software can facilitate new computing infrastructures and how the synergy of a fresh, diverse team can be harnessed to span the divide between computational and experimental research in engineering and science. A web-based data repository will serve as a communication hub among the partners to allow instant access to all tools and findings. After validation, these methods will be made available to the scientific community at large through the same hub. Incorporating this research into courses taught at the partner universities will inform future computational scientists and experimentalists how to build a highly interactive collaboration that accelerates discovery and innovation.

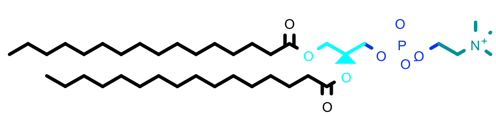
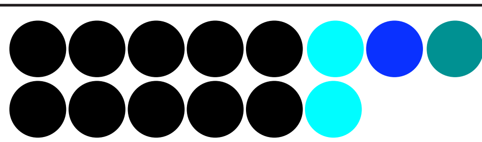
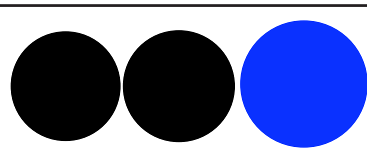
Perhaps the single most important scientific challenge of the project is overcoming the multiple length scales in the computational studies required to effectively predict the ultimate properties of the nanoparticle stabilized liposomes. Liposomes are lipid bilayer vesicles of 20–500 nm diameter, which translates to surface areas of 63–1570 nm2. While simulations of liposomal behavior have been performed on the sub-nano (atomic and molecular level), nano, and meso scales (**Table 1**), approaches that focus on any one scale are insufficient for designing the nanoparticle stabilized vesicles. Sub-nano simulations are essential for informing the design of suitable organic molecules to tether the vesicle to the nanoparticle core and molecular level insight for interpreting experimental data. However, nano and meso scale modeling are essential for predicting the particle stability and dynamic properties of the entire nanoparticle assembly. Hence, generating new design knowledge by intelligently combining the wealth of existing data and techniques will be crucial for overcoming the challenges of multiple length scales.

In order to better illustrate the concept of length scales, one can consider the challenge of modeling the phospholipid bilayer that envelopes the liposome. Ideally, synthetic chemists would want the molecular-level details afforded by atomistic modeling to accurately predict the properties of each phospholipid molecule present within the ultimate nanoparticle stabilized liposome. Through application of knowledge about the relationship between structure and specific liposome properties suitable molecules could be synthesized efficiently. Unfortunately, the large number of molecules present in a liposome would require extremely long computational times following an atomistic approach.

Table 1 illustrates the concept for a typical lipid component of a bilayer membrane. The atomistic model of the lipid contains 130 atoms, each described by a mathematical function. A typical simulation may use 144 lipids plus 11,200 water molecules. Using the fastest supercomputer, simulating 1 nanosecond of "molecular time" takes 2 days. Even with 144 lipid molecules, the simulation is too small to model entire liposomes, and would be unable to probe phenomena such as large-scale bending of membranes, phase behavior, and interactions with colloids. However, meso-scale modeling can actually simulate these properties. As depicted in Table 1, this modeling sacrifices atomic details by reducing the phospholipid into cruder representations to allow shorter computational times. The computational savings allow modeling with more "molecules" that represent a larger surface area of the membrane for longer periods of time. The Cooke—Deserno model describes the lipid molecule with 3 spheres, whereby a complete spherical liposome can be studied computationally for 1 millisecond. Of course, the cruder model means that the ability to rationally synthesize new molecules would be sacrificed. Fortunately, nano-scale modeling provides the ability to bridge atomistic and mesoscale modeling. The MARTINI model in Table 1 represents the lipid molecule with 14 spheres (mathematical functions that represent the properties of a group of atoms). The key feature of these simulations is their ability to reproduce the results of both atomistic and mesoscale modeling that help verify that the models are reasonable.

Figure 1 sets the approach for the project, which requires a transdisciplinary team with theoretical and experimental expertise ranging from chemistry to biophysics to soft matter physics. This team approach will solve a complex challenge while training young engineers and scientists. These young engineers and scientists will augment their primary training with hands-on experience in all four laboratories. As such, this project will produce researchers, who, in the spirit of the ICTAS mission, will "engage in . . . research at the intersection of engineering, science, biology, and the humanities to advance the frontiers of knowledge . . .". With a lot of hard work and good fortune, this team just might construct a nanoparticle that can solve a long-standing medical challenge.

Table 1. Different scales for simulations illustrated for a lipid molecule

Model (scale)	Depiction	surface area range	simulated time range
Atomistic (sub-nano)		0–25 nm2	0–100 nsec
MARTINI (nano)		0–250 nm2	0–1 μsec
Cooke-Deserno (meso)		0–2.5 μm	0–1 msec

Introducing the 2009 ICTAS Doctoral Scholars

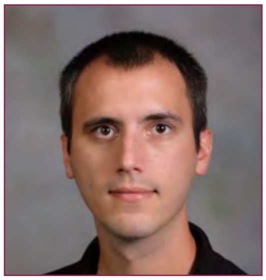
Sarah Foltz is a Ph.D. student in the department of Biological Sciences at Virginia Tech and an ICTAS Doctoral Scholar. She is advised by Dr. Ignacio Moore of the Ecology, Evolution, and Behavior group.

Sarah grew up in the San Francisco Bay Area of northern California and received her Bachelor's degree from the University of Washington in Seattle. Her research is field-focused, which compliments her love of the outdoors. Her interests include horseback riding, hiking, and camping, as well as making art from found and recycled materials and reading anything she can get her hands on.

Sarah is broadly interested in how organisms adapt to new and challenging environments through physiological and behavioral mechanisms. As a corollary to this, she is also interested in the function and conservation of natural variation within populations.

Benjamin Gordon Freedman is a Ph.D. candidate in the Department of Biological Systems Engineering, concentrating in Bioprocess Engineering, and is advised by Dr. Ryan Senger. Benjamin's research interests are in the area of combinatorial methods for metabolic engineering in microorganisms to optimize biofuel production. Benjamin's research activities have so far been diverse, including industrial paper production, naval systems research, and toxicology studies aboard NASA's "Weightless Wonder" C-9 aircraft.

Benjamin comes to Virginia Tech from Caribou, Maine, where he enjoyed skiing, running, hiking with his dog, and classical literature.



Gregory James is a Ph.D. student in the Department of Chemical Engineering at Virginia Tech, and an ICTAS Doctoral Scholar. He is currently working on his initial classroom preparatory work for his qualifying exams and is awaiting the assignment of a research advisor in the latter part of the fall semester 2009.

Gregory comes to Virginia Tech from Chesapeake, VA and is now residing in Christiansburg, VA. When he is not in the lab, his interests include golf, hiking, cycling, and disc golf. He is currently planning to take a cross-country cycling trip upon the completion of his doctoral degree. At home, Greg likes to cook and spend time with his wife and friends.

Greg's research interests include fuel cells, polymers, and surface chemistry.

Jeong-Ah Lee is a Ph.D. student in the Department of Physics at Virginia Tech, and an ICTAS Doctoral Scholar. She is currently advised by Dr. Victoria Soghomonian, Associate Professor, Department of Physics.

Jeong-Ah is from Seoul, South Korea. Other than physics, her passion lies in music, especially classical music and jazz. Her

:: NEWS BRIEFS ::

Helping hand

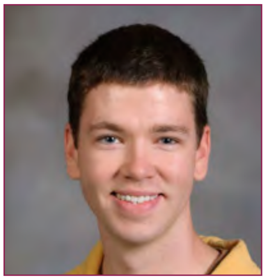
Dr. Tom Campbell, Associate Director for Special Projects, facilitated a Humboldt Kolleg entitled "Nano-Bio: The Next Transformative Convergence." (Pictures on page 15)

Bringing it all together

ICTAS will celebrate one year of occupancy of the ICTAS headquarters building in March 2010. The first annual ICTAS RESEARCH DAY is among events planned and will include renowned technology experts, keynote talks, building tours, lab demonstrations, a poster session, food, giveaways and more.

favorite classical music composer is Chopin and she enjoys playing the romantic pieces on piano. She wants to learn jazz piano as well. She is also interested in movies and building miniatures.

Jeong-Ah's research interests are in condensed matter physics, especially nanoscale science and devices. Recently, she gave an oral and poster presentation on "Various Methods of Producing Suspended Graphene Structures for NEMS Applications" during the 10th International Conference on the Science and Application of Nanotubes (NT09) in Beijing, China.



Taylor Mach is a Ph.D. student in the Department of Chemistry at Virginia Tech and is advised by Dr. Daniel Crawford. Taylor received B.S. degrees in Chemistry, Biochemistry/Molecular Biology, and Biology from Bethel University in 2009.

Taylor is from Inver Grove Heights, Minnesota. In his spare time he enjoys riding his motorcycle, playing soccer, watching House, and reading science fiction novels.

His research experience and interests involve using high performance quantum chemical methods to study topics ranging from interstellar chemistry to the electronic excited states of radicals. He's also interested in the implementation of computational methods on large multiprocessor computers.

William (Bill) Vogt is a Ph.D student in the Virginia Tech–Wake Forest University School of Biomedical Engineering and Sciences. He works in the Biomedical Optics and Devices Lab under the supervision of Dr. Christopher Rylander. Bill's research is related to the study and finite-element modeling of the mechanical, thermal, and optical properties of human skin. The results of this work can then be used in design of devices for diagnostic and therapeutic applications.

Bill, a resident of Millis, Massachusetts, received his Bachelor's degree in Mechanical Engineering, summa cum laude, from the University of Massachusetts – Amherst. As an undergraduate, Bill wrote a thesis studying the combination of feedback controller design and drug administration protocol, sparking his current interest in the fusion of engineering and biology. When away from the lab, Bill passes the time with music, be it singing, woodwinds, or piano.

The ICTAS Doctoral Scholar Program was established in 2007 to honor exceptional beginning Ph.D. applicants through award of financial support for the Ph.D. qualifying period. This program is a cooperative effort supported and coordinated primarily by ICTAS, with significant contributions from participating departments, colleges and the Graduate School. Nomination may be made through departmental graduate coordinators within the partner colleges including engineering, science, agriculture and life sciences, natural resources and veterinary medicine.

Partnership is our business

VT President Charles Steger and Captain Sheila Patterson (shown at left), celebrate the recent signing of a five-year, $7.5 million indefinite delivery/indefinite quantity contract and a Cooperative Research and Development Agreement (CRADA) between Virginia Tech and the Naval Surface Warfare Center Dahlgren Division (NSWCDD).

Pipe infrastructure management systems: bridge over academic studies and practical applications

Tae Il Park | Postdoctoral Associate | taeil09@vt.edu

For the last 30 years, the need for expanding and upgrading sewer systems has dramatically increased in response to a need to meet the dramatic growth of communities. Because of this dramatic growth and the lack of timely information about systems' performance, most sewer systems operate in a reactive mode and allocate most of the system resources to the rehabilitation or complete replacement of already failed systems. In response, government agencies are paying more attention to the implementation of infrastructure management systems, which will allow governmental agencies to manage and improve sewer systems efficiently and cost-effectively during the entire life of the asset.

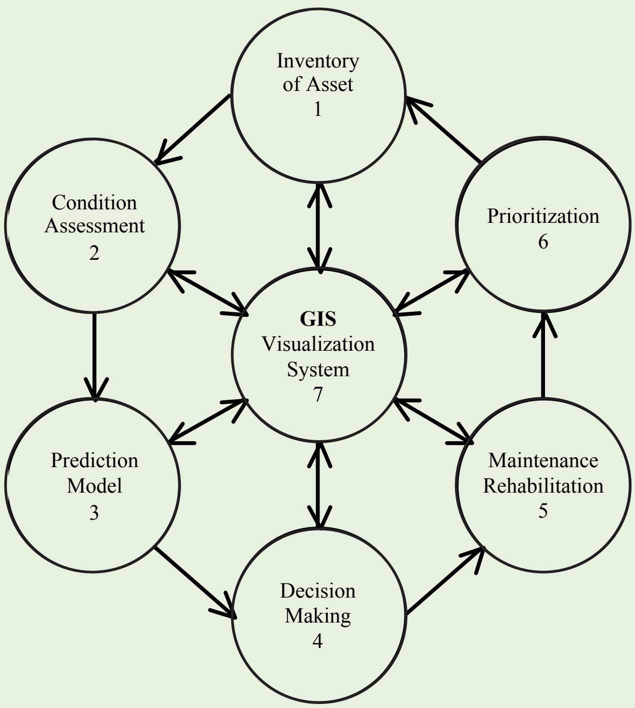
Infrastructure management is a systematic approach that guides the maintenance, operation, preservation and improvement of infrastructure assets to obtain optimum service delivery and resource allocation throughout the infrastructure's service life. Overall, the ICTAS Center of Excellence for Sustainable Water Infrastructure Management (SWIM) involves entire components of an infrastructure management system including establishment of nation-wide databases, construction of generalized condition rating system, prediction modeling of pipe behavior, decision making for rehabilitation and replacement of the system, etc.

Taeil Park joined the SWIM team in July 2009 with a charge to expedite the field of prediction modeling. Park earned his degree in comprehensive sewer infrastructure management systems and also has competitive background in Markov chain-based prediction modeling, asset valuation, dynamic programming, fuzzy logic theory and real option.

Currently, Park is planning to propose an originative and practical way to identify possibility of system failure and its consequence. While conventional prediction modeling estimates performance of a system directly, using historical data which is not readily available, The approach proposed by Park investigates the influence of surrounding conditions such as soil condition, average daily traffic, ground water table, properties of pipeline etc. on the behavior of system and anticipates the service life of system indirectly. This project clearly identifies critical parameters for the deterioration process and also explains the deterioration mechanism of the system. Overall, this project will assist governmental agencies in establishing long-term investment plans and budget allocations.

Park's overarching goal as a member of SWIM is the establishment of a complete infrastructure management system which could be easily utilized by state and local agencies. He believes that simplicity and easiness of the infrastructure management system would be the first step to bridge the gap over academic studies and their application in real world.

Park earned his master's degree from the University of Southern California and a Ph.D. from Pennsylvania State University under Dr. Sunil Sinha who is currently an Associate Professor and Director of the ICTAS Center for Excellence in Sustainable Water Infrastructure Management.



Overview of Infrastructure Management System

Welcome recent additions to the ICTAS team

Anna Furry, Receptionist | 231-2597 | acfurry@vt.edu

Furry recently completed an honors B.A. in Interdisciplinary Studies at Virginia Tech. She brings with her to ICTAS varied background experience that was gained through employment during her college years including employment as a regional representative for the Orthodox Christian Fellowship, a restaurant associate, and a museum curator.

Jon Greene, Program Manager, CNavS | 231-8566 | greenej@vt.edu

Greene comes to Virginia Tech after concluding a twenty eight year career with the military, most recently as the Commanding Officer of the Naval Surface Warfare Center, Dam Neck, Virginia Beach, VA, where he led a 350 person research and development organization focused on systems of systems integration, interoperability and integrated training capabilities. Greene earned a M. A. in National Security Affairs from the Navy Postgraduate School and a B.S. in Political Science from the United States Naval Academy. He has served as a member of the Armed Forces Communications and Electronics Association, the U.S. Naval Institute, the National Defense Industry Association and the Hampton Roads Technology Council.

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Park earned a Ph.D. in civil engineering from Pennsylvania State University. While serving as a research assistant at PSU, Park developed a valuation model for sewer infrastructure, two-step optimization process for rehabilitation and replacement policies, and investigation of deterioration process of sewer pipelines. Park's current research interests are focused on the asset management system of sewer infrastructures including prediction model, valuation model, and decision process.

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Schroedl is a graduate of the Virginia Tech Computer Engineering department. He brings information technology customer service experience gained through positions as a computer technician intern and helpdesk technician to ICTAS. Additionally, Schroedl is a Microsoft Certified Professional , A+ Certified Professional and Network* Certified Professional.

Autumn Timpano, Lab Facilities Manager | 357-0514 | aclapp@vt.edu

Timpano brings significant lab experience with her to ICTAS, some of which was gained in Virginia Tech laboratories. Timpano previously served as a laboratory technician in the Department of Biological Sciences at Virginia Tech, a fermentation microbiologist in the Virginia Bioinformatics Institute at Virginia Tech and as a quality assurance microbiologist with Valleydale-Gwaltney-Smithfield Foods, Inc. Timpano earned a B.S. in Biology at Virginia Tech.

Advancing Water Production Processes for Future Generations

Chris Cornelius | ICTAS Associate Director for Research | chcornel@vt.edu

Cornelius

__Chris Cornelius__ is an associate professor of chemical engineering, associate director of the Institute for Critical Technology and Applied Science (ICTAS), and the technical director of the Center for Naval Systems at Virginia Polytechnic Institute and State University. As a senior research administrator of ICTAS for Virginia Tech, he shares responsibility in the strategic research investment of $8MM/yr in the areas of Water, Energy, Renewable Materials, Nanomaterials, and National Security. He has over 13 years of experience associated with the synthesis and characterization of polymers, sol-gel chemistry, hybrid organic-inorganic materials and ionomers at Sandia National Laboratories and industry. His research efforts have resulted in numerous collaborations with industry, National Laboratories, and university researchers throughout the nation.

Introduction

The unifying focus of Cornelius's research emphasizes the development and understanding of polymers, hybrid organic-inorganic materials, sol-gel chemistry, and organically templated sol-gel "self-assembled" materials. Research interests include the creation of membrane materials for gas separations, proton exchange membranes for hydrogen and methanol fuel cells, anion-exchange membranes for water electrolysis, and proton and anion exchange membranes for water desalination via electro-dialysis, reverse osmosis, and alkaline fuel cells. Currently, Cornelius is actively working towards developing new water production technologies as part of an emphasis on water sustainability research at ICTAS.

Who needs it?

The answer is that we all need it. Fresh, potable water is an essential human need and increasing water shortages threaten the world's peace and prosperity. Improved water technologies are needed as water shortage problems increase throughout the world. For example, population growth in the US is expected to increase 13.6% per decade with the simultaneous growth to China and India. The challenge for our civilizations is that only 0.5% of the Earth's water is suitable for human consumption. The remaining water is in our oceans as saltwater or locked up in glaciers and icecaps. As the world's population grows, the increased water demand will have to come from somewhere. Waste water, brackish water, and seawater have great potential to fill the coming requirements. Unfortunately, the ability to exploit these resources is currently limited in many parts of the world by both the cost of the energy and the investment in equipment required for purification/desalination.

The beginnings of membrane based desalination took place nearly a century ago and the improvements in desalination based reverse osmosis (RO) technology over the last 25 years is represented in Figure 1.[1] Future solutions are needed for producing fresh water "economically" as populations and agricultural demands continue to grow. In order to maintain the sustainability and security of our national water infrastructure and meet future drinking water standards, the development of inexpensive and efficient water production processes are required. RO is recognized as an effective method for water desalination and removal of a wide variety of organic and inorganic contaminants. RO is believed to be one of the key technologies for future water production, but current RO systems suffer from inorganic and biological fouling at membrane surfaces that reduces water flux, processing robustness, and increases the cost of producing fresh water.[2] In order to minimize these deleterious effects, elaborate water preconditioning steps are done in order to prevent scaling and biofouling in a RO modules. RO systems require significant pretreatment steps to prevent premature membrane failure due to biological and inorganic fouling. Even with these limitations, RO is one of the leading desalination technologies used in the world.

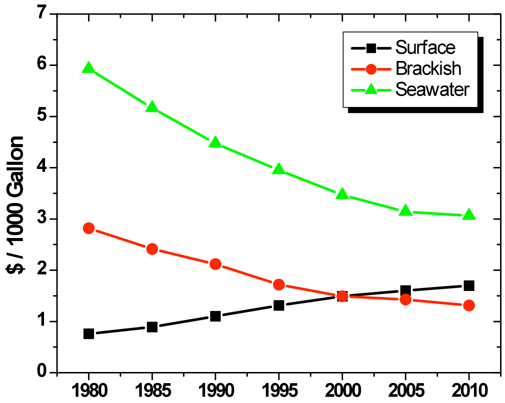
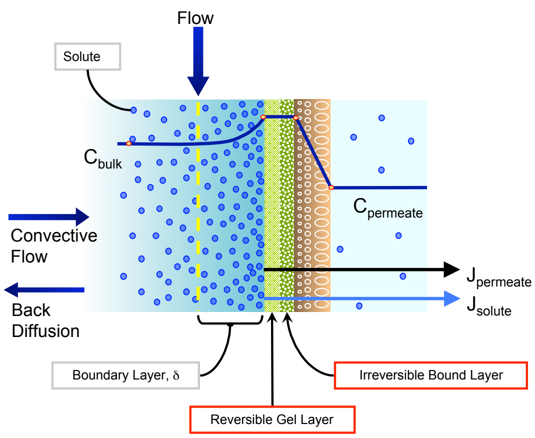


Figure 1. Reverse-Osmosis desalination cost trends for producing 1000 gallons of water.[3]

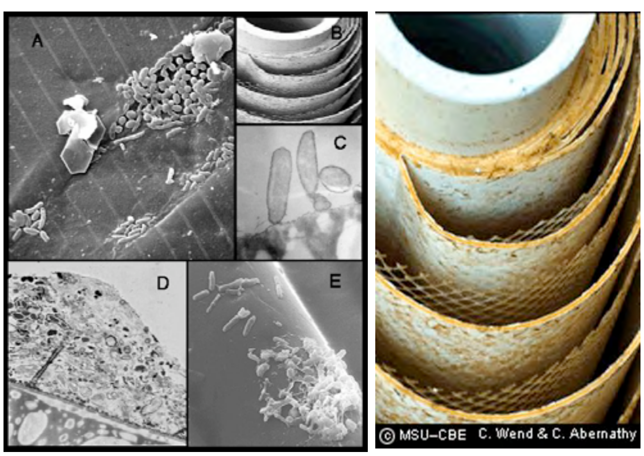
Cornelius Seeks a Solution through Water Desalination – Reverse Osmosis (RO) Research

RO is a leading water treatment technology for water desalination with costs decreasing over the last 25 years.[4,5] However, significant technical challenges exist with RO membranes due to the complexities of surface waters. One desalination challenge is the formation of a reversible gel layer that becomes irreversible due to biofouling by bacteria. The process of membrane biofouling begins when bacteria excretes an exopolymeric substances (EPS) that is used to terraform a surface in order to make it suitable for cellular growth. In order to minimize these deleterious effects, elaborate water preconditioning steps are done to prevent biofouling.[6,7] Figure 2 is an idealized representation of the dynamic bio-fouling process from reversible bacteria adsorption to bacteria colony growth.

Figure 2

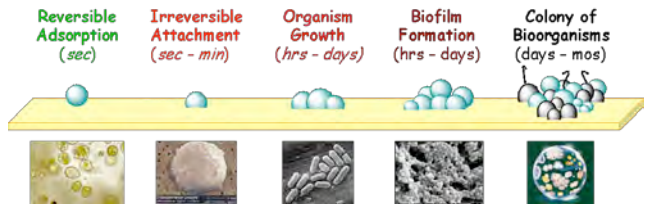


▲ *A) Water flux through a RO membrane with gel layers and salt concentration gradient.*

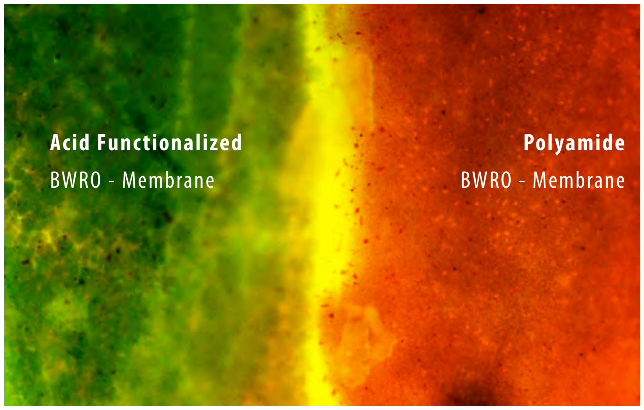


▲ *B) Example of bio-fouling in RO membranes.*

Figure 2 (continued)



▲ *C) Bacteria adsorption to colony growth as a function of time.*



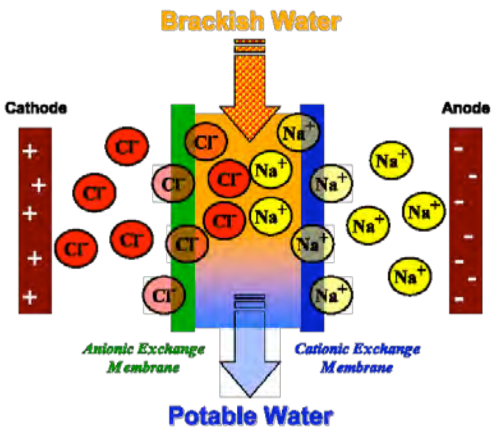
▲ *D) Mitigation of bacteria growth on a RO membrane using an ionomer to create a functional coating.*

While membrane type affects water transport and salt rejection, it also influences bacteria adsorption. Several of these membrane and solution interactions arise from ionic, steric, dispersion forces, polar/non-polar properties of the material, and the water environment. These factors all contribute to salt rejection characteristics and tendency to foul by biomatter, organics, and inorganics. Solutions to these challenges will be realized by advancing polymer structure, morphology, selective transport, and membrane surface properties in order to mitigate biological and inorganic fouling.[8] Figure 2 has initial results of Cornelius's work illustrating that ionic charge can be used to inhibit biofouling on a surface. Continuing research efforts in water treatment will be centered on the fundamental study of surfaces and material science as it relates to water and ion transport, biofouling, and salt rejection in novel membranes.

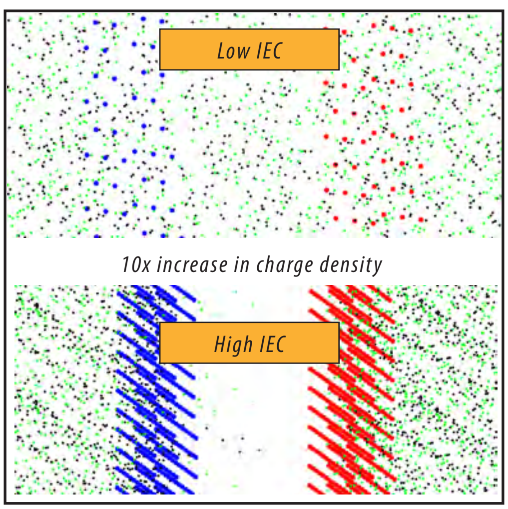
Water Desalination – Electro-Dialysis (ED)

The theoretical energy for removing ions from water is identical for all desalination processes. Observed desalination differences are due to the methodology of mass transport through the membrane for ED and RO. ED is recognized as the most cost-effective method for desalinating brackish waters even though this technology has not undergone significant advances in over 30 years.[9] Utilizing Donnan Exclusion, ED selectively transports and rejects ions using an electric potential and oppositely charged anionic and cationic membranes (Figure 3). A significant opportunity exists for advancing ED through the design of new ionomers that improve selective transport of charged ionic species. Cornelius's initial research efforts in designing and testing anion exchange membranes (AEMs) have shown a 50% improvement in the rate of desalination due to enhanced ion transport. These results illustrate the tremendous impact on the improving transport with engineered materials. Cornelius's ongoing research focuses upon the molecular design of ionomers for the improvement of ED desalination and controlling ion transport.

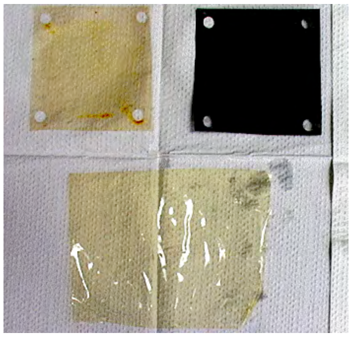
Figure 3



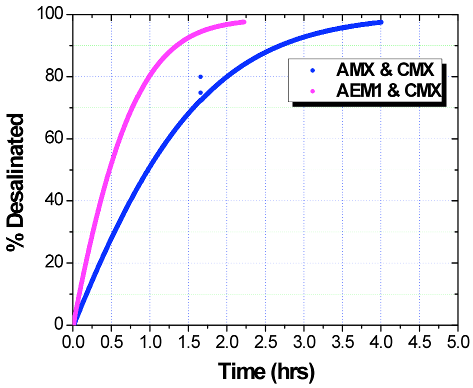
▲ *A) Functional overview of ED and salt transport.*



▲ *B) Salt rejection as a function of ion exchange capacity (IEC) – molecular modeling done by Sandia National Laboratories.*



◀ *C) Ionomer structure of AMX versus AEM Gen1 and stability in a 1M NaOH solution.*



◀ *D) Desalination rate of AMX membranes versus AEM Gen1 membrane (2X faster).*

Conclusion

Developing an advanced water production processes will enhance the nation's ability to ensure safe clean water for future generations. This research addresses the technical and economic challenges of desalinating water and it directly contributes to the research vision of developing new desalination technologies as described by the Desalination Technical Roadmap developed jointly by Sandia National Laboratories and the US Bureau of Reclamation. It is anticipated that several new insights from this research will arise in the areas of desalination, modeling, polymer anti-fouling strategies, and separations necessary for establishing new insights in science and engineering.

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◀ Images from a **Humboldt Kolleg**

This two-day conference, October 14 - 15, assembled world leaders in Nano-Bio to exchange ideas, present latest findings, provide networking opportunities, and charter fruitful directions for future research.

▼ **ICTAS II:** Putting the Pieces Together

Construction of the ICTAS II Building on Virginia Tech campus continues to move along. Anticipation is building for the new possibilities it will provide.

ICTAS RESEARCH AWARDS

Congratulations to 2009 mid-cycle research award recipients.

ICTAS awarded support for four (4) additional research projects in a second wave of funding decisions for 2009. These awards are based on selected proposals that were submitted in response to the 2009 ICTAS request for proposals (RFP).

Team Leader	Title
J. Socha	Biomimetic Microsystems Inspired by Physiological Networks in Insects
J. Freeman	Conductive Biocompatible Nanoactuators
J. Holliday	Exploiting Natural Genetic Variation to Improve Wood Properties and Biomass Yield in Poplar
M. Zhang	Proof of Concept Study of Carbon Nanohorn Supported Virus Envelope-like Particles as Novel Vaccines

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Ann Craig, editor | Alex Parrish, graphic designer

Dr. Roop Mahajan, Director, Institute for Critical Technology and Applied Science, discusses research collaboration with Dr. Regina Dugan, newly appointed Director of the Defense Advanced Research Project Agency (DARPA), during her visit to Virginia Tech on August 27, 2009. Dugan earner bachelor's and master's degrees in engineering from Virginia Tech before earning a doctorate from the California Institute for Technology.

: : News Briefs : :

Glimpsing the Light – ICTAS Scientific Report

Fall semester activities 2009 include publication of the first ICTAS Scientific Report. The report includes individual project reports of progress achieved through seed or early stage research funded by ICTAS and performed during the last fiscal year.

Destination: Future

The ICTAS Academy of Interdisciplinary Research is formed to serve as a catalyst to attract the best and brightest distinguished scholars to a collaborative and stimulating atmosphere in ICTAS for the science and practice of interdisciplinary research. The academy recognizes individuals who have made outstanding contributions through teaching, research, practice and design, or a combination of such activities.