

## Focus on Energy

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By 2030, the world is expected to use more than 678 quads of energy per year, nearly double the annual energy use just ten years ago. This increase in energy use is attributable to worldwide population growth and to economic development in countries such as China and India as they seek to achieve living standards comparable to those currently enjoyed by western nations. The economic, environmental, and societal impact of this increase is likely to be dramatic. For example, by 2030, annual petroleum demand is forecast to be more than 25% higher than the annual demand in 2008 when oil prices reached \$150 per barrel.

While new resource discoveries and new energy technologies are likely, the fact remains that changes in our energy infrastructure occur very slowly with time scales on the order of decades. The development of hybrid vehicle technology provides a useful example. In 1999, the first hybrid vehicles were met with great market demand and widespread enthusiasm. The popularity, availability, and annual sales of hybrid vehicles has grown steadily over the years. And yet, after ten years, hybrid vehicles constitute less than 1% of the US light duty vehicle fleet. Similarly lengthy technology

deployment cycles could be cited for other energy systems such as advanced technology power plants (e.g. gas turbine combined cycle plants), solar power, emission control technology, next generation nuclear plants, and others. Thus, if we are to meet the world's energy challenges two decades from now, it is imperative that we begin to make changes today.

In the US, we face two principal energy challenges – (1) the development of economical, environmentally benign alternatives to the petroleum fueled internal combustion engine for the transportation sector and (2) the development of generation technologies with reduced environmental impact for the electrical utilities sector. Together, these two sectors account for more than 80% of US primary energy use and 74% of CO<sub>2</sub> emissions. Though often conflated, these sectors are essentially disconnected and present dramatically different challenges. The transportation sector is comprised of millions of small independent energy conversion devices operating almost exclusively on petroleum derived fuels with more than 60% of the fuel supplied by non-domestic sources. The transportation sector presents environmental challenges, economic challenges (due to rising global petroleum demand), and strategic challenges (due to the lack of alternatives to imported petroleum). On the other hand, the utility sector is comprised of a relatively smaller number of very large interconnected energy conversion systems operating on a variety of fuels almost all of which are domestic in origin. Due to the abundance of domestic resources for producing electricity, the primary challenge in the electricity sector is mitigating environmental impact.

Understanding the urgency of the energy challenges that we face, ICTAS is focused on accelerating discovery, development, and deployment of technologies that can contribute to solving challenges in either the transportation or electrical generation sectors. A particular focus of our work has been



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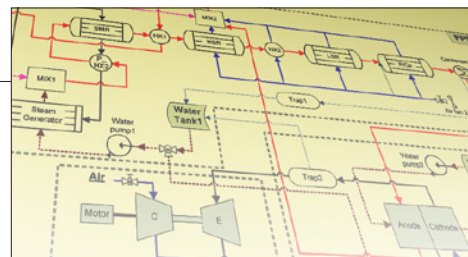
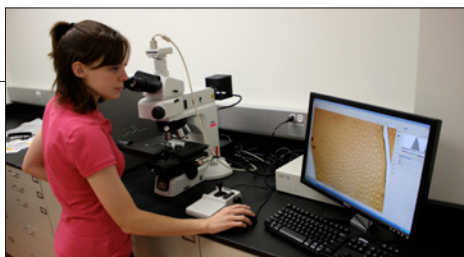
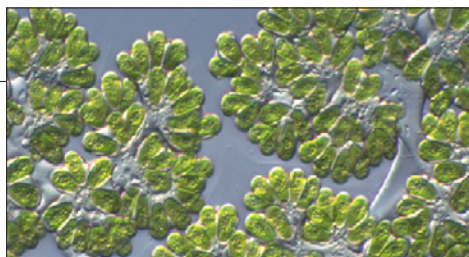
the development of biofuels that can provide alternatives to petroleum for transportation. Currently, there are more than 7 million flex fuel vehicles on the road capable of using E85 (a blended fuel comprised of 85% ethanol and 15% gasoline). This number represents roughly 3% of the US vehicle fleet and is already considerably larger than the fleet size expected for battery electric vehicles at the end of the decade. Thus, there is a substantial opportunity to displace petroleum with ethanol using the existing vehicle fleet. However, the production of ethanol by current technologies yields a more expensive product than gasoline and can create competition for agricultural resources that are used to produce food. ICTAS supported research has sought to develop alternative feedstocks that are more amenable to biofuels production and to develop novel processing technologies that use a wider range of feedstocks and that improve overall crop-to-tank economics. These efforts, led by professors Foster Agblevor, Bingyu Zhao, Chenming Zhang, and Percival Zhang are described in the Biomass to Fuels article on page 6 and the Enzymatic Conversion article on page 7.

While the development of biofuel alternatives to petroleum is essential to improving economics and security in the transportation sector, biological sources by themselves cannot meet current transportation energy needs. A joint DoE/USDA study suggests that biomass resources could provide up to one billion tons of feedstock, sufficient to displace up to 30% of our nation's petroleum use, without dramatic changes in agricultural practices. Thus, it is essential to improve automotive efficiency to reduce petroleum dependence in the short term and to better align our needs with available resources should we move to reliance on biofuels or other renewable sources over the long term. Automotive fuel cell technology can increase efficiency, improve fuel source diversity, and reduce local emissions while supporting the trend toward increasing electrification of the vehicle power train. ICTAS affiliated research, supported by a mix of government and industry funding, has led to advances in fuel cell materials, fuel cell material characterization techniques, and predictive modeling of fuel cell performance and durability. This work, involving professors Jim McGrath, David Dillard, Scott Case, Robert Moore, Doug Nelson, Michael von Spakovsky, and Michael Ellis is discussed in more detail in Fuels-to-Electricity article on page 8.

In the electrical power sector, the application of solar photovoltaic (PV) technology for the direct conversion of sunlight to electricity has long been an appealing goal, but the adoption of solar power has historically been limited by the high cost of PV modules. However, since 1980, the price of PV modules, in real dollars, has declined by nearly a factor of ten. And, in 2008, a major US solar panel manufacturer achieved the long-sought goal of manufacturing PV modules at a cost of less than \$1/Watt. Manufacturing costs this low lead to solar power installations that produce electricity at costs competitive with grid electricity in high-cost markets (e.g. California and several of the northeastern states). Further improvements of roughly 2-3 times, achieved through reductions in manufacturing cost, auxiliary component cost, distribution cost, and/or installation cost can make solar power competitive with grid electricity in most regions of the US.

The PV module cost, in \$/Watt, is determined by the manufacturing operations used to produce the modules and by the cell efficiency, which determines the module size required to produce a specific amount of power. Research supported by ICTAS, seeks to develop organic solar cell technology that dramatically reduces manufacturing costs and to develop silicon-based multi-junction solar cells that dramatically improve efficiency. Organic solar cells produce electricity using polymer based materials that can, in theory, take advantage of the high-volume, low-cost manufacturing techniques developed for the polymer production and processing industries. Research in this area has been led by professors, Randy Heflin, Harry Dorn, Harry Gibson, and Robert Moore and relies on novel materials and nanoscale assembly techniques developed at Virginia Tech. This work is described in more detail on page 10. Research in the area of multi-junction solar cells is led by Professor Mantu Hudait who joined Virginia Tech in 2009. His work is featured in the Faculty Focus section on page 12.

Energy affects almost every area of our lives. The development of energy technologies to meet society's future needs must therefore engage a wide range of scientific and engineering expertise. The ICTAS team welcomes input and participation in our research efforts as we seek to develop a more sustainable energy future.



*Key areas of sustainable energy research at ICTAS include: renewable energy resources (e.g. solar and biomass); cleaner more efficient energy conversion systems (e.g. fuel cells, enzymatic transformation), and source-to-application integration for improved sustainability.*



# ICTAS: Helping Us Meet Society's Needs



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The Institute for Critical Technology and Applied Science (ICTAS) is contributing to Virginia Tech's international recognition for research in: nanoscale science and engineering; molecular and cellular biology; sustainable development, including energy, water and renewable materials; and cognition and communication. Its goal to engage faculty and students in interdisciplinary and collaborative research across engineering and the physical and life sciences will allow Virginia Tech to make greater strides in meeting the future needs of society.

As the world's population grows and its countries become more developed over the next 40 years, food production must increase significantly and may, in fact, need to double. Along with this increased food production is the need to accomplish this feat with environmentally sustainable systems that use no

additional energy, water, and land than is used today. Development of such systems will require new discoveries and the development of new methods to produce, store, process, and distribute food. During this same time frame, the need for health and disease research will grow with the growing population.

The College of Agriculture and Life Sciences is positioned well to contribute to these challenges. In fact, Virginia Tech's research expenditure in agricultural sciences for 2008 was ranked by the National Science Foundation at #5 among US universities and colleges. Much of the College's research is focused on food and agricultural productivity and environmental sustainability, biodesign and bioprocessing, and health and disease.

Meeting global challenges will require faculty members and students to work across disciplines, much like ICTAS is fostering. For example, faculty members in the Department of Biological Systems Engineering are working across the College of Engineering and the College of Agriculture and Life Sciences to combine biological, chemical and engineering principles to produce food, fuels, pharmaceuticals, and other biomaterials in ways that conserve and protect our natural resources and the environment. The applications of new genetic advances in the plant and animal sciences, new techniques for processing and storing food products, and new health-related advances in nutrition, food and exercise will benefit from interdisciplinary teams. Many faculty members are also affiliated with the Cooperative Extension Service where many of their discoveries can be further studied and then applied to society.

The interdisciplinary activity in ICTAS also creates an environment that is conducive for the development of scientists who we rely on for creativity and future innovations. We must prepare those who can also link new discoveries in basic research programs to practical applications in society. We must prepare scientists who are strong in single disciplines, but who are effective at working across disciplines. The grand challenges of the future will require interdisciplinary teams composed of members that are experts in their disciplines, yet have the ability to work effectively with members of other disciplines. ICTAS is positioned well to help address these grand challenges.



# Harvesting Energy for a Sustainable Future



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In an address before a Joint Session of the Dail and Seanad, Dublin, Ireland, June 28, 1963, President John F. Kennedy remarked that "The supreme reality of our time is the vulnerability of the planet." Perhaps nowhere is this vulnerability more critical than in the availability of sustainable energy sources now and into the future.

The ICTAS **Sustainable Energy research thrust** is organized to develop and promote energy –related research and solutions across the university through advancing discovery and scholarship. This special issue of the ICTAS newsletter captures some of the exciting and relevant research under this thrust area. In the lead article, Professor Michael Ellis provides a framework in the context of solving energy challenges in the transportation and electrical generation sectors. This introduction is followed by in-depth key articles on a spectrum of technologies describing the multi-faceted approaches to energy conversion. Other ICTAS-supported supplementary and complementary research efforts, underway but not covered in this newsletter, include those under the umbrella of the ICTAS Center for Energy Harvesting Materials and Systems (CEHMS) and the ICTAS Center for Clean Coal Energy (IC<sup>3</sup>E). Led by Professors Dan Inman and Shashank Priya, CEHMS has been successful in generating interest from several companies seeking products such as self-powered wireless sensor networks in structural health monitoring and distributed power sources in unmanned vehicles. CEHMS currently has four industrial members and recently fulfilled all the requirements necessary to become a full-fledged NSF I/UCRC.

A generous one million dollar donation from Appalachian Energy Power (AEP), spurred the formation of IC<sup>3</sup>E, in conjunction with an established research program in clean coal energy under the leadership of Professor Srinath Ekkad. Prof. Ekkad, in collaboration with Prof. Roe-Hoan Yoon, has initiated a large effort on campus to reduce the carbon footprint of existing fossil-fuel-based power

plants. This effort is also supported through the DOE National Energy Technology Laboratory. Discussions of these and other energy-related research efforts will be included in a subsequent issue of this newsletter.

I would also like to take this opportunity to welcome Dr. Alan Grant, Dean, College of Agriculture and Life Sciences, to the ICTAS Stakeholder Board. He brings a wealth of rich experience in teaching, research, outreach, and administrative accomplishments, the benefit of which he shares with us in the context of his message included on the previous page of this newsletter.

Finally, in the November 2009 issue of the ICTAS Connection (<http://www.ictas.vt.edu/pdf/conn7.pdf>), I described the ICTAS concept of strategic investing over an extended period of time to "grow our interdisciplinary research, not in a straight line, but instead in an upward spiral." A key element of this strategy is allocating a portion of our resources to promoting blue sky thinking that might lead to disruptive technologies of the future. Recently, ICTAS launched a new seminar series entitled "The Black Swan and Disruptive Technology." In the NY Times best seller, *The Black Swan*, the author (Nassim Nicholas Taleb) defines a Black Swan as an event that has three characteristics: it is an outlier; it carries an extreme impact; it has retrospective predictability. While it may not be possible to predict the next Black Swan, it is my contention that we can create an environment and a breeding ground for future Black Swans – an environment in which engineers, scientists and humanists from different disciplines can come together to move beyond predictable and incremental advances in current technologies to the disruptive technologies of the future. We plan to use this forum to imagine the next transformative technologies in the harvesting and deployment of energy for a sustainable future as well as other areas acknowledged by experts as major challenges to society's sustainable future.

# Facilities Updates

## ICTAS (Headquarters location on campus at Stanger Street)

Moving into a newly constructed or renovated building is the culmination of a complex undertaking, involving a spectrum of activity from land acquisition to architectural drawings, to the first shovel of earth to the first step on the fresh flooring. The final product is a major investment and asset.

As of March 2010, faculty, staff, students and visitors have enjoyed one year of occupancy of the headquarters building. The building is fully occupied and brimming with activity. Tenants include:

- First floor – CIB; SWIM; Energy and Material Transport; Targeted Delivery of Nanomedicine; Cognitive Radio Network
- Second floor – Biobased Materials; Environmental Nanoscience and Technology; Targeted Delivery of Nanomedicine
- Third Floor – School of Biomedical Engineering and Sciences (SBES)
- Fourth Floor – ICTAS Administration; Sustainable Energy; Carbonaceous Nanomaterials.



## ICTAS – CRC (Virginia Tech Corporate Research Center location)

The Nanoscale Characterization and Fabrication Laboratory (NCFL), located on the first floor of the ICTAS-CRC building, is currently in the third year of operation. A recent addition to the NCFL, the Varian MR400 MHz NMR system, provides basic molecular structural information used to characterize new materials and guide the synthetic process. This capability is provided as part of ongoing research efforts for Dr. Theresa Reineke (Biorganic and Polymer Chemistry), and Dr. Timothy Long (Polymer Chemistry).

The ICTAS/SBES Advanced Multi-scale CT Facility continues to expand under the direction of Drs. Ge Wang and Chris Wyatt. By bringing together various state-of-the-art CT scanners to a common area, the Multi-scale CT allows improved access to CT scans at various spatial resolutions – ranging from mm to sub 50nm.

Over the next four years Virginia Tech scientists will be involved in a National Science Foundation project to build six additional SuperDARN radars. Virginia Tech has unique responsibilities within the SuperDARN international collaborative network of high frequency (HF) space weather radars including software development, database management, web-based outreach and data distribution. The SuperDARN group originally came to the VT campus in April 2008 and recently acquired additional space in the NCFL to accommodate growth over the last two years.



## ICTAS-LSC (Life Sciences Corridor campus location)

Construction at the LSC location began in April 2009 and is currently 60% complete. The current project scope includes enough points to obtain a LEED Silver certification, making this the first research building on the Virginia Tech campus to gain LEED certification. Substantial completion is slated for year-end 2010 and occupancy is expected early in 2011.



## ICTAS-NCR (National Capital Region Ballston location)

ICTAS will expand 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 7,000 square feet in this facility. The anticipated construction completion date is April-May 2011.





# Biomass to Fuels

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## Biomass feedstock modification for efficient biofuels production

Natural biomass feedstocks are composed of lignin, cellulose, hemicelluloses and extractives. Although these polymeric constituents are potential raw materials that could be converted to various types of biofuels, their natural structures are such that they are very difficult to process efficiently to higher value products. The major challenges are the accessibility of the biopolymers to enzymes and other chemicals, multiplicity of products generated from the degradation of the biomass, toxicity of treated biomass to biocatalysts, and high oxygen content of the biomass which results in low energy density. Further, because biofuels are commodity chemicals and have low energy densities, they are currently not competitive with energy dense fossil fuels. One proposed method of improving profitability of the biomass is to genetically modify the biomass feedstock to produce active pharmaceutical proteins in addition to the biomass. These pharmaceutical proteins will be extracted first, and then the residual biomass can be converted into biofuels. Because the pharmaceutical proteins have very high value, they will make the entire process economically viable and competitive with fossil fuel production.

The processability of the biomass feedstock can be improved through plant breeding and genetic modification. Breeding and genetic modification can generate new plants with either high lignin or cellulose contents. Genetic tools can also be used to transform the biomass to improve accessibility to enzymes and chemicals. One such approach is the introduction of cellulose degrading enzymes into the plant in a dormant state and activating the enzymes to degrade the biomass after the harvest.

During the past year we commenced two research programs to improve the quality of the biomass feedstock for efficient processing. 1. Breeding of new lines of drought tolerant and disease resistant switchgrass; 2. Transformation of switchgrass to express endoglucanase enzymes.

## Breeding of switchgrass lines

About 158 lines of switchgrass were generated in the greenhouse and screened for various properties. These plants have varying properties in terms of biopolymer composition, physical properties, disease resistance, and drought tolerance. We are developing rapid analytical methods to screen these feedstocks for further processing. Currently, rapid pyrolysis and thermogravimetry analysis methods are being used to screen the biomass feedstocks. The preliminary thermal analysis results showed strong variation

in chemical composition among the feedstocks. Further, the feedstocks also showed strong variation in their resistance to grinding. Some feedstocks were easy to grind, whereas others were very difficult to grind. We plan to correlate these properties with efficiency of converting the feedstocks to biofuels.

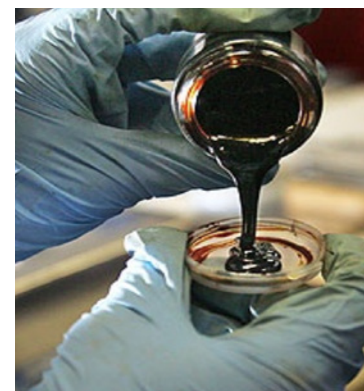
## Genetic transformation of switchgrass

We investigated the transformation of switchgrass to express endoglucanase enzymes. This is a model system to eventually express active pharmaceutical proteins into the switchgrass feedstock. In the proposed approach, the proteins will first be extracted and then the residual biomass will be converted to biofuels. We successfully transformed the switchgrass to express endoglucanase enzymes in the leaves of the plantlets. The plantlets are being grown in the greenhouse to generate enough biomass for further processing to show proof of concept.

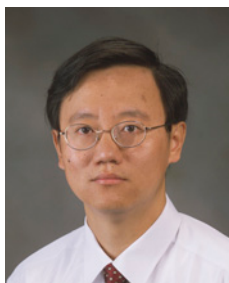


*Switchgrass provides a wide range of versatility for the future of biofuels.*

-- Collaborating Researchers: Dr. Foster Agblevor, Dr. Bingyu Zhao, Dr. Chenming Zhang, Dr. Changhe Zhou



*Stable pyrolysis oil produced from biomass.*



# Enzymatic Conversion: Simpler is Better

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## Enzymatic Conversion - Simpler is Better: Cell-free Systems from Scientific Study to Biofuels Production

Living organisms exhibit remarkable abilities for transforming energy from one form to another through complicated enzymatic networks but they insist on growing and duplicating themselves. By identifying and combining key enzymes for desired products but not including those for self-duplication, we can mimic and even improve upon these conversion pathways. Synthetic biology is an emerging field that integrates engineering, chemistry and biology to create transformative biologically inspired pathways for extracting energy and synthesizing materials. In affiliation with ICTAS and other sponsors, including the Air Force Office of Scientific Research, Dr. Percival Zhang is working to develop an in vitro assembly of purified enzymes and coenzymes capable of producing low-value biofuels with very high yields. Using a cell-free approach called Synthetic Pathway Biotransformation (SyPaB), this research has demonstrated the conversion of starch or cellulosic materials to hydrogen at a yield of nearly 12 moles of hydrogen per mole of glucose, the highest value in the world. Moreover, the demonstrated process is a low temperature endothermic process, which can be easily integrated with other energy system components to utilize waste heat streams. The ultimate goal of the work is to develop a fuel cell vehicle that operates on hydrogen derived from safe, high energy density sugars stored on-board. With the improved reaction rates associated with the enzymatic conversion process as well as the improved efficiency of fuel cell power plants relative to their conventional competitors, Dr. Zhang estimates that the 2050 US light-duty transportation needs can be met by ~600 million tons of dry biomass annually.

While enzyme deactivation remains a challenge, several stable enzymes with total turn-over numbers (TTNs) of more than  $10^8$  have been obtained. If this TTN could be realized for all of the enzymes, estimates suggest that hydrogen production costs would be as low as \$1.50 per kg, where a kg of hydrogen

has roughly the same energy content as a gallon of gasoline. Current focus areas for the production of hydrogen from biomass sugars using synthetic biology include (1) developing thermostable enzymes for use as building blocks in cell-free SyPaB, (2) modifying enzymes that can work on more stable low-cost biomimetic cofactors, (3) accelerating hydrogen generation rates and (4) demonstrating more SyPaB applications from sugar batteries to biohydrogenation.

-- Collaborating researchers: Dr. Percival Zhang, Dr. Jonathan Mielenz at Oak Ridge National Laboratory, Dr. Mike Adams at University of Georgia



### Reference:

Zhang, Y.-H.P. A sweet out-of-the-box solution to the hydrogen economy: Is the sugar-powered car science fiction? *Energy Environ. Sci.* 2, 272-282 (2009).



# Fuel-To-Electricity

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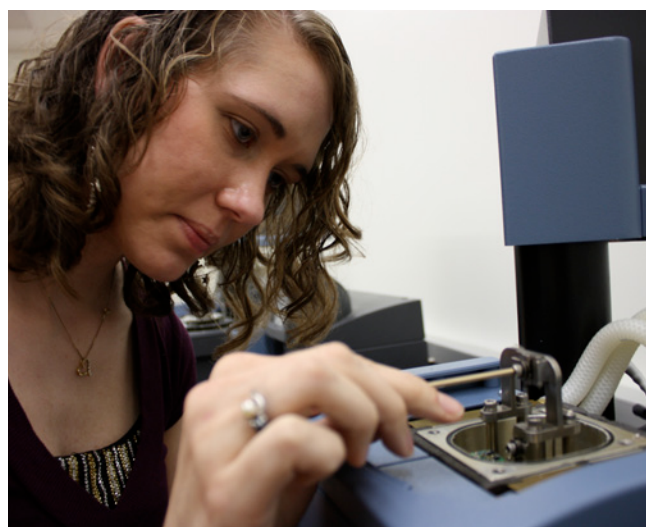


Future transportation energy needs will likely be met through a portfolio of sources rather than exclusively by petroleum. Electric vehicles, biofuels, and hydrogen are particularly promising options for fueling personal transportation vehicles. Although hydrogen should be seen as an energy storage medium rather than a source, the high energy density, good energy conversion efficiency, emission of nothing but water vapor from hydrogen-powered vehicles, and other promising features have led many to see tremendous opportunities for an entire economy based on hydrogen generation, delivery, and use.

Recognizing the potential of hydrogen fuel cells for automotive and other applications, a significant effort in fuel cell technology has been underway at Virginia Tech for the past decade. This work has involved synthesis and processing, of new materials, development of material characterization techniques, modeling of performance and durability, and development of novel components and systems. Several groups in both the College of Science and College of Engineering have been involved. Much of our fuel cell work has involved polymer electrolyte membrane (PEM) fuel cells, which are of specific interest for transportation and portable electronic applications. James McGrath, University Distinguished Professor and Ethyl Corporation Chair of Chemistry, has pioneered several new polymeric membrane materials offering significantly lower cost, greater resistance to methanol crossover (for methanol fuel cells such as might be useful for personal portable power requirements), and improved durability. Donald Baird, Alexander Giacco Chair of Chemical Engineering, along with others have developed techniques for making bipolar plates that could be used between the individual cells within a PEM fuel cell stack.

In addition to new materials, the success of PEM fuel cell technology will require the development of cell components with predictable, long-term durability. Recognizing the importance of durability to the future of PEM technology, a team of researchers located in the ICTAS Sustainable Energy Laboratory has been engaged in industry-funded research to study the durability of membrane and seal components for these systems. Professors Scott Case, Michael Ellis, Robert Moore, and David Dillard are now in the 5th year of an intense collaborative research effort with General Motors being directed by Dr. Yeh-Hung Lai (VT, Ph.D. 1994) of General Motors. This ICTAS-

affiliated research project has brought over a million dollars in research support to the group, funding their efforts to develop characterization techniques, test methods, and durability prediction capabilities for perfluorosulfonic acid (PFSA) and perfluorocyclobutyl (PFCB) membranes. Working closely with Dr. Lai and his colleagues at GM, our group has pioneered the development of a viscoelastic framework for characterizing, predicting, and understanding membrane durability. Morphological studies are providing insights into the complex nature of the membranes, how their properties are affected by processing variables, and how these changes may affect the durability of these membranes under the demanding environments experienced by membranes within operating fuel cells. Constitutive characterization of the viscoelastic properties and hygrothermal swelling of these membranes provide essential information for predicting the stresses that result in constrained membranes subjected to the cyclic hygrothermal conditions within a fuel cell. The group has successfully demonstrated the utility of the time temperature superposition principle for correlating constitutive data collected over the relevant temperature range, but has also shown that hygral and stress or strain-based shifts can be used to incorporate the effects of moisture content



*ICTAS researcher Katherine Finlay characterizes the mechanical response of materials for PEM fuel cells*



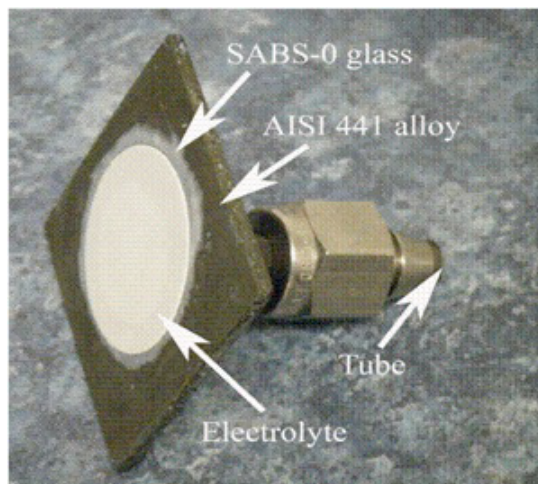
and applied stress or strain levels. Novel membrane strength characterization techniques have been developed based on the use of pressurized blister tests, providing the first mechanical loading method for PEM materials in which laboratory tests can detect the types of leakage damage than can result in reactant gas crossover failures encountered in fuel cell operation. Successful implementation of these techniques allows us to detect damage from ramp-to-fail, static fatigue (creep), and cyclic fatigue loadings. Knife slit techniques have been developed to characterize the fracture resistance of the membranes, information that may be important in understanding durability. Finally, these characterization techniques and the results they have generated have been incorporated in lifetime prediction methodologies that are providing valuable information for estimating life and performance of PEMs under complex operational cycles. We are especially pleased with the significant amount of technology transfer of techniques to our sponsor through this collaborative project, which has been significantly facilitated by ICTAS.

In addition to membranes, other polymeric materials are required for PEM fuel cells. In a Department of Energy funded project led by UTC Power, members of the Sustainable Energy Laboratory team have been involved in durability studies of elastomeric materials for seals required to prevent mixing of reactive gases in PEM fuel cell stacks. Professors Scott Case, John Dillard, Robert Moore, and David Dillard are involved in this effort. Durability studies of a hydrocarbon-based seal material produced by Henkel have been underway for the past three years. Viscoelastic properties of both the elastomer and of seals prepared with relevant cross-sections have been characterized through dynamic mechanical analysis (DMA) and stress relaxation tests conducted on subscale molded o-ring specimens (SMORS) at several temperatures and in a range of environments. Additional tests have been conducted on tensile and tear specimens to characterize the effects of these environments on the durability of these seal materials and the seal geometry being studied. This interdisciplinary project has resulted in the development of several test techniques; results obtained have led to improvements in material durability; and test results are providing guidance on the life such materials might exhibit in fuel cell applications.

In addition to our work in the area of material characterization and durability for hydrogen fueled PEM fuel cells, researchers affiliated with ICTAS have developed novel PEM fuel cell architectures and explored the use of microbial fuel cells for the production of electricity from organic wastes. Low temperature, PEM fuel cell systems have traditionally utilized stack configurations in which cells are assembled face-to-face in series to form a rectangular block. These block configurations are not always compatible with the shapes of products requiring fuel cell power. Research led by Professors Michael Ellis and David Dillard and supported by Ecolectrix, LLC., has sought to develop planar PEM fuel cell configurations for application in flat shapes such as miniature aircraft wings and electronics packages. In addition, Professors Michael von Spakovsky and Michael Ellis in conjunction with Luna Innovations have explored the development of flexible microtubular fuel cells which can

be conformed to fit spaces available within small unmanned vehicles. Finally, ICTAS researchers have begun to explore the use of exoelectrogenic bacteria as anode catalysts in microbial fuel cells (MFCs). These bacteria can oxidize organic material, such as that occurring in wastewater streams to produce electrical power. An initial ICTAS affiliated project funded by the Water and Environmental Resources Foundation (WERF) and led by Professors Nancy Love, Ishwar Puri, and Michael Ellis demonstrated more than an order of magnitude improvement in microbial power production when stainless steel anodes were enhanced by the addition of flame synthesized carbon nanostructures. Currently, Professor Bahareh Behkam is leading an ICTAS research effort to understand the role of surface characteristics in promoting microbial attachment and power production in MFCs. This work has applicability for energy recovery from wastewater treatment as well as energy harvesting for powering remote monitoring systems.

While much of the ICTAS fuel cell effort has focused on relatively low temperature ( $<100^{\circ}\text{C}$ ) fuel cells, we have also explored the development of solid oxide fuel cell components which operate at temperatures exceeding  $800^{\circ}\text{C}$ . The solid oxide fuel cell research has been led by Professors Michael von Spakovsky and Kathy Lu. Professor von Spakovsky has developed a suite of numerical techniques for describing SOFC electrode pore structure and for modeling the transport of contaminants within this structure. Professor Lu has developed a novel SOFC seal glass that can prevent leakage from the cell assembly while accommodating the high stresses imposed by thermal cycling of the SOFC stack. The seal glass has been tested for sealing ability with heating rates of  $3\text{--}20^{\circ}\text{C}/\text{min}$  for 2500 hrs and 100 thermal cycles with excellent performance. Her group has also initiated new research for fuel cell material interfacial interaction and degradation. Professor Lu's work has been supported by the US DoE through their Solid State Energy Conversion Alliance program and by the Idaho National Lab.



*AISI 441/SABS-0 glass/ZrO<sub>2</sub> tri-layer assembly for sealing test. The SABS-0 glass was developed by Virginia Tech researchers.*

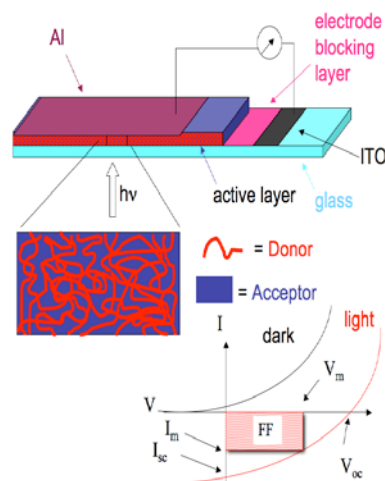
# Sunlight-To-Electricity

by James R. Heflin | Professor, Physics |  
540-231-4504 rheflin@vt.edu



Worldwide production of oil is forecast to peak ~2030. In the search for alternative energy sources, efficient utilization of solar energy is an appealing approach. Current photovoltaic technology uses silicon as the primary material for solar energy conversion, with a typical power conversion efficiency of ~12% and a cost that is currently 2-3 times more expensive than fossil fuels. Organic photovoltaic materials are of great interest because of the potential to enable inexpensive, lightweight, flexible devices with improved solar conversion efficiency.

In an ICTAS Grand Challenge Project, Profs. Randy Heflin (Physics), Harry Dorn (Chemistry), Harry Gibson (Chemistry), and Bob Moore (Chemistry), along with their graduate students Manpreet Kaur, Hunter Champion, Daniel Schoonover, and Scott Forbey, are developing the next generation of polymer solar cells. Plastic solar cells, consisting of blends of conducting polymers and fullerenes, are under intense investigation as alternatives to silicon-based systems. In these devices, light is absorbed by the polymer causing excitation of an electron to a higher energy level. Without the presence of the fullerene (such as the buckyball  $C_{60}$ ), the electron simply returns to its original lower energy level and the polymer re-emits the energy as fluorescent light. However, if there is a fullerene within 10 nm of the excitation site, the electron will be transferred to the fullerene yielding a separated electron and hole, where the hole consists of the missing electron on the polymer chain. Polymer solar cells have great potential in view of their expected lower cost and mechanical durability and flexibility. However, the best present organic polymer-based cells, at ~5% efficiency relative to ~12% for commercial silicon cells, are hampered by



*Schematic of a bulk heterojunction organic photovoltaic device and a plot of I-V responses in the dark and light. Important variables are  $I_m$ , the current at maximum power;  $I_{sc}$ , the short circuit current;  $V_m$ , the voltage at maximum power;  $V_{oc}$ , the open circuit voltage; and FF, the fill factor.*

1) lack of understanding and control of the nanoscale morphology of the composite system and 2) lack of proper alignment of the energy levels of the donor and acceptor. Regarding morphology, the team has been developing an approach wherein a concentration gradient of the donor acceptor components is achieved to maximize the concentration of the majority carrier

component in the vicinity of each respective electrode while maintaining close proximity of the donor and acceptor species. This has been accomplished through sublimation of a  $C_{60}$  layer on top a spin-cast polymer layer followed by thermally-induced interdiffusion of the two films. With respect to the energy levels, they have begun exploring incorporation of endohedral metallofullerenes, which have lowest unoccupied molecular orbital (LUMO) levels >0.4 eV higher than that of the conventionally used PCBM fullerene derivative. The increased LUMO level should result in a >50% increase in the open circuit voltage and, correspondingly, power conversion efficiency of organic solar cells.



*Manpreet Kaur in the photovoltaics lab*

# Welcome recent additions to the ICTAS team



**Moanaro Biswas, Postdoctoral Associate** | 231-6032 | [naro79@vt.edu](mailto:naro79@vt.edu)

Biswas came to Virginia Tech from the National Institute of Immunology, New Delhi, India, where she performed research as part of projects entitled "cross-regulation of macrophage apoptosis by HIV-Nef and mycobacteria" and "studies on the regulation of immune responses to Japanese encephalitis virus infection." Biswas will work with Dr. Elankumaran Subbiah in the Center for Molecular Medicine and Infectious Diseases.



**Janet Murphy, Fiscal Tech Senior** | 231-9930 | [jrmurphy@vt.edu](mailto:jrmurphy@vt.edu)

Murphy began Commonwealth of Virginia employment as a fiscal assistant with the Southwestern Virginia Mental Health Institute. In August 2005, Murphy transferred to Virginia Tech Dining Services and in 2006 joined Aerospace and Ocean Engineering. Previous work experience includes work in the private sector in accounts payable and receivable. Murphy's duties with ICTAS include payroll forms processing, wage payroll actions, travel reimbursement, and secondary contact for Hokie mart actions.



**Deborah Aruguete, Postdoctoral Associate** | 231-3058 | [aruguete@vt.edu](mailto:aruguete@vt.edu)

Deborah Aruguete came to Virginia Tech in 2006 as a Postdoctoral Research Scientist to explore fate/impact of man-made nanomaterials in the environment. Deborah works with Dr. Michael Hochella, University Distinguished Professor of Geosciences, on projects including bacteria-nanoparticle interactions and nanoparticle dissolution. Effective March 25, 2010, Deborah became Associate Director of the VT SuN Center.

# Congratulations and well wishes to Chris Cornelius

Chris Cornelius, Associate Director for Research for the Institute for Critical Technology and Applied Science, has accepted a faculty appointment as Associate Professor of Chemical Engineering at the University of Connecticut located in Storrs, CT commencing with the fall semester 2010. The state's flagship institution of higher education with an enrollment of nearly 30,000 undergraduate and graduate students, is part of a University system that includes 10 Schools and Colleges at its Storrs campus, separate Schools of Law and Social Work in Hartford, five regional campuses throughout the state, and the Schools of Medicine and Dental Medicine at the UConn Health Center in Farmington.

Cornelius came to ICTAS in 2008 from Sandia National Laboratories, a National Laboratory operated for the U. S. Department of Energy by Sandia Corporation. In the role of Associate Director for Research with the Institute for Critical Technology and Applied Science, he served as chief technical officer and advisor to institute Director Roop Mahajan, sharing responsibilities for technical administration, setting strategic directions, and allocating resources on behalf of the institute while continuing as an active researcher in synthetics and materials.

Significant reshaping of the ICTAS research structure was accomplished under

Cornelius's leadership through strategic resource investment in research and creative input to research team development. Cornelius served as principal author of proposals that resulted in the establishment of the first ICTAS national security partnerships with the Naval Surface Warfare Center Division at Dahlgren (\$9.5M contract award) and the Advanced Propulsion Laboratory (\$1.5M contract award) as well as an ICTAS center devoted to continuing responsiveness to national security concerns. Cornelius also contributed to the enhancement of external recognition of ICTAS through development of the first ICTAS Scientific Report, preparation of research and administrative reporting data, and development of information for sharing through website and publications.

"Although I am looking forward to new challenges and alliances, I am also feeling some sadness about leaving Virginia Tech and all of the wonderful friends and colleagues established here," Cornelius mused.



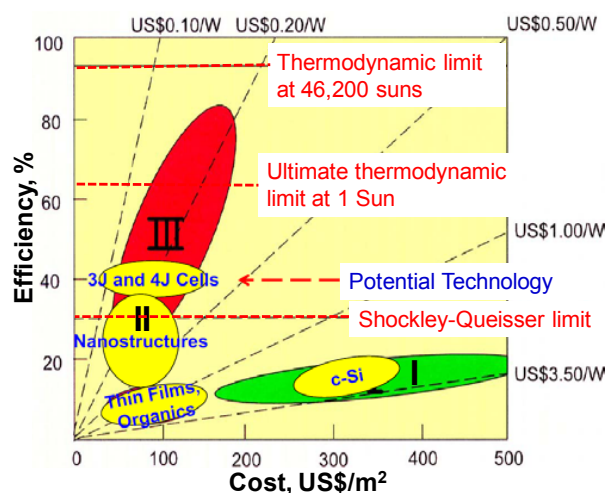


# Multijunction III-V photovoltaics and thermophotovoltaics on large area, low-cost silicon substrates for alternate energy solution

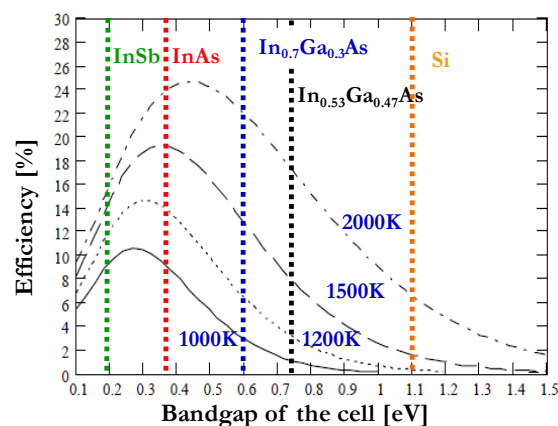
by Mantu Hudait | Associate Professor, Electrical and Computer Engineering |  
(540) 231-6663 | mantu@vt.edu



Given the looming global energy crisis and environmental challenges, including concerns with climate change and fossil fuel shortage, we need to develop alternative sources of renewable energy (1-5). Photovoltaics (PV) and thermophotovoltaics (TPV) conversion of solar and thermal energy is a clean method for producing electricity that does not produce any (net) carbon dioxide emission. The co-generation of electricity from thermal energy are said to be quiet, reliable, clean and efficient. The energy demand and the electricity generation from renewable energies, particularly from PV and TPV are comparatively higher costs today and that are inhibiting the wide-spread dissemination of renewable energies and needs to be cheaper at cost/watt. Solar energy and TPVs are one of the prime sources of renewable energy and also prime candidates for research and development. There remain two main challenges for PV and TPV for wide spread dissemination: one hand i) to reduce the cost of material by exploring novel materials, new device structures to discover new physical mechanisms for energy conversion onto cheaper large area substrates, and on the other hand ii) to enhance the conversion efficiency in order to reduce the cost per watt. Novel discoveries and innovations potential lead to high-efficiency power sources for future electronic systems. The outcome from our research efforts on multijunction photovoltaic cells incorporated with quantum wells and quantum dots as well



**Fig. 1:** Efficiency vs. cost of photovoltaic technology. The biggest challenge is dramatically reducing the cost/watt to deliver solar electricity (6).



**Fig. 2:** Efficiency versus bandgap of cell as a function of black body radiator temperature.

as low bandgap thermophotovoltaic devices heterogeneously integrated onto large area, low-cost silicon substrates will be the key enabler of producing electricity for wide spread dissemination. Our research thrust falls within the University's strategic priority area of "Energy, Materials, and Environment". This indicates Virginia Tech's commitment to research in sustainable energy, in this case addressing the need to provide electricity at an affordable cost per watt. Virginia Tech and ICTAS have recognized the tremendous value that new sustainable energy can bring to our nation and is committed to being a leader in research in this discovery domain. Higher efficiency with lower cost/watt is a significant challenge for solar energy conversion. Fig. 1 shows the efficiency versus cost of PV technology and the biggest challenge is drastically reducing the cost/watt to deliver solar electricity. The III-V compound semiconductor in a 3 or 4 junction cells in a monolithic multijunction form having multiple semiconductor layers with different bandgaps demonstrated higher efficiency and this could be the potential technology in future. Besides the potential for high efficiency, III-V semiconductor compound materials have advantages including the bandgap tunability by elemental compositions, higher photon absorption by the direct bandgap energies, higher resistivity against high-energy rays in space, and smaller efficiency degradation by heat than Si solar cells. In fact, energy conversion efficiencies around 40% under solar concentrators of 236-454 Sun and 27% under AM0 have been recently achieved utilizing InGaP/InGaAs/Ge triple junction concentrator configuration (3-5) and the cell thickness of four junction cell in excess of 10 $\mu$ m (4) prohibits

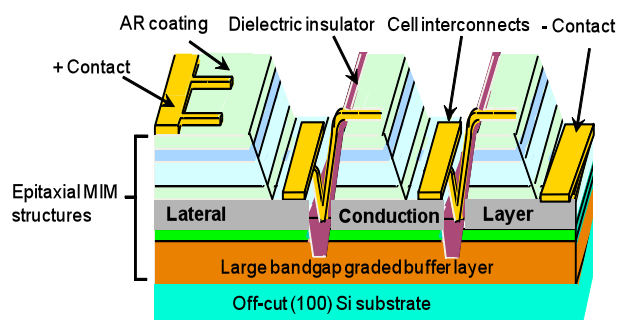
the enabler of economy-of-scale production. An alternative approach is to grow quantum well (QW) and quantum dot (QD) structure inserted into the intrinsic region of a host cell offers a theoretical conversion efficiency of about 63% (7), where the total thickness of the multijunction cell is less than 5µm or (ii) the triple junction cell structure onto lattice engineered, low-cost and large area silicon substrate to address the cost/watt. Cheap and readily available silicon wafers in sizes from three to eighteen inches may be the key enabler of economy-of-scale production of solar cells.

Thermophotovoltaic energy conversion is a direct thermal-to-electric energy conversion process whereby an emitter or radiator is heated to incandescence and a photovoltaic device is placed in view of the emitter. Incident photons from thermal energy of sufficient energy are converted into electrical energy by the photovoltaic device. For efficient operation, up to 75% of the radiant energy from the emitter needs to be recycled for a TPV system with a moderate temperature broadband emitter (1200K to 1500K) and a low-bandgap photovoltaic device ( $0.5\text{eV} < E_g < 0.75\text{eV}$ ) (8-11). The principle of TPV is the same as in solar PV cells, except that the source for TPV applications is much closer and has a temperature of around 1500-2000K rather than the 5800K of the sun. As the black-body spectrum is given by Planck's law:

$$\rho(\lambda, T) = \frac{2\pi hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda kT}} - 1},$$

the peak wavelength  $\lambda_p$  shifts with temperature T according to Wien's law  $\lambda_p = 2.898 \times 10^6 \times T^{-1} \text{ nm K}$ . The infra-red radiation is therefore of greater interest in TPV applications instead of the visible part of the spectrum for solar cells. Using the radiative limit, the theoretical efficiency limit of a single band-gap cell as a function of band-gap is shown in Fig. 2 for several black-body spectra. Therefore, the efficiency can be increased by increasing the blackbody temperature or in the multijunction form of the TPV cells, similar to the concept of multijunction concentrator solar cell configuration.

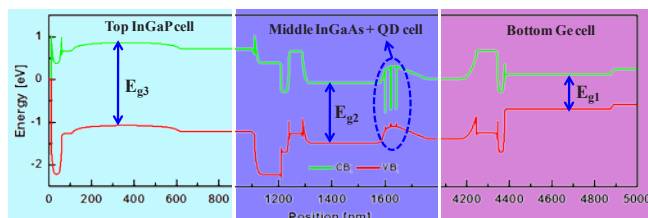
A main focus of our research work at Virginia Tech is to develop a (i) multijunction III-V tandem solar cell structure incorporated intermediate band (IB) QDs or QWs inside the host cell, (ii) the triple junction III-V tandem cell structure, and (iii) low bandgap TPV devices onto Si substrates. Incorporating these QDs or QWs into multijunction III-V solar cell provide a means of adjusting the absorption edge of the component junctions and thus increasing the short-



**Fig. 3: Schematics of the monolithic integrated module (MIM) of TPV devices.**

circuit current. Further, by using alternating compressive and tensile materials, a strain balanced QD or QW solar cell stack can be grown defect free, providing absorption-edge/lattice parameter combinations that are inaccessible using bulk materials. Careful interface engineering and device design utilizing QD and QW provides an attractive way to achieve multijunction cells with optimum bandgap profiles that do not suffer from lattice mismatch induced defect degradation. In order to become a viable technology solution, the serial architecture of monolithically grown photovoltaics require: i) current matching of each cell; ii) transportation of carriers between cells; iii) higher minority carrier diffusion length; iv) low-loss and highly-doped tunnel junction, which produce an effective potential barrier for minority carriers; v) desired doping of each layer; vi) low defect density to avoid recombination of carriers; and vii) lower overall processing and materials cost per watt. Similarly, careful interface and device engineering and monolithic integrated module (MIM) of TPV devices (10, 11) onto the large area, low-cost Si substrate as shown in Fig. 3 will be a key enabler for producing highly efficient thermal energy conversion devices and also to avoid developing very expensive large diameter III-V substrates. Heteroepitaxial growth of III-V on Si involves complex material issues such as, polar-on-nonpolar growth, lattice mismatch, chemical mismatch and thermal mismatch. These problems typically result in poor crystalline quality due to formation of various defect types such as anti-phase domains, misfit and crystal defects such as threading dislocations, twinning and stacking faults. Should such integration succeed, it would open new vistas for low-power and high speed logic, alternate energy solution, chip-to-chip or on-chip communication and sensing applications. Our research programs are addressing these issues at Virginia Tech.

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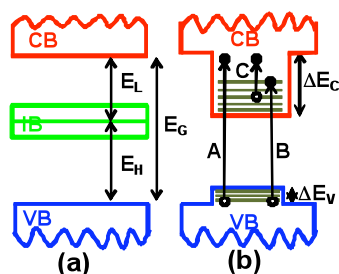


**Fig. 4:** Simulated band diagram of triple junction lattice matched InGaP/InGaAs (+InAs 3-QDs)/Ge heterostructure solar cell.

### Multijunction QD solar cell

Fig. 4 shows the simulated energy band diagram of one of the triple junction cell design with 3-InAs QDs embedded into InGaAs middle cell on Ge substrate. The insertion of multiple InAs QD layers into InGaAs cell forms an isolated intermediate band within the bandgap of the InGaAs cell, the efficiency of the cell can be exceeded to Shockley-Queisser limit (12) of 31% at AM0 condition. Absorption of photons with energy below the InGaAs bandgap occurs from InGaAs valence band to a partially occupied IB formed by InAs QD and from IB to InGaAs conduction band, thereby increasing the photocurrent by the additional  $VB \rightarrow IB$  and  $IB \rightarrow CB$  absorptions, as shown schematically in Fig. 5. As these low energy photons are normally lost in a standard cell, the QD approach will enhance the current gain by extending the absorption spectrum of the nanostructure solar cells and hence the efficiency. The InAs QDs on InGaAs will form in the Stranski-Krastanov growth mode and measures must be taken in order to prevent the generation of the misfit and threading dislocations due to strain relaxation. The bandgap of the InGaAs quantum dot system can be tailor-made to tune the solar spectrum of the nanostructure tandem solar cell configuration.

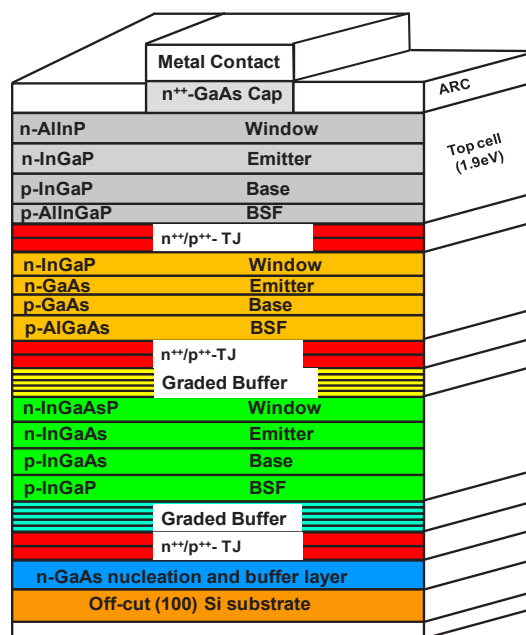
Multijunction III-V solar cell: The InGaP/GaAs/InGaAs metamorphic structure of



**Fig. 5:** Schematic diagram of single-particle energy levels in a QD array and its equivalent intermediate-band system: (a) valence band (VB), conduction band (CB), and intermediate band (IB); (b) desired transitions.

triple junction solar cell on Si substrate is shown in Fig. 6. Our research group has recently acquired a molecular beam epitaxy (MBE) growth system with in-situ reflection high energy electron diffraction capability will allow us to investigate the growth mechanism, defect generation issues due to mismatch and interface control of GaAs on Si as well as latter in the solar cell structure. With my previous experience at Indian Institute of Science (India), Ohio State University and at Intel Corporation, our research will develop a next generation III-V multijunction solar cell structures, low bandgap gap TPV devices, and III-V based low-power logic structures, all will be heterogeneously integrated onto large area, low-cost Si substrates.

With the past experience on the multijunction solar cells (13-16), III-V materials growth, quantum well device structure and device results on Si substrates (17-20), and MBE system for materials and device structure growth, state-of-the-art equipments available at ICTAS, device process facilities that available at Virginia Tech, our research group will develop multijunction photovoltaic and thermophotovoltaic device structures for wide spread dissemination at an affordable cost/watt.



**Fig. 6:** Schematic cross-sectional diagram of a multijunction tandem solar cell structure on lattice engineered silicon substrate.



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# AEP Foundation Support of ICTAS Sustainable Energy Research

ICTAS energy research efforts are currently supported by a generous donation from the American Electric Power (AEP) Foundation. The AEP Foundation donation of \$1 million provides support for post-doctoral associates working in the fuel cell, bioenergy, and clean coal areas and support for the purchase of additional equipment for our Sustainable Energy Laboratory. The ICTAS team looks forward to working with these postdoctoral associates to make significant advances in ICTAS research programs. Mr. R. Daniel Carson, Jr., Vice President of Appalachian Power, a subsidiary of American Electric Power, was instrumental in identifying the opportunity for the AEP Foundation to support energy research at Virginia Tech and worked with Ms. Deborah Hamilton at the Virginia Tech Foundation to make this donation a reality. Mr. Carson is a professional engineer, a former member of the College of Engineering Advisory Board and a 1970 Civil Engineering graduate of Virginia Tech. The AEP Foundation gift is in honor of Joe Vipperman, retired Executive VP of AEP and former President of Appalachian Power. Joe was one of the original ICTAS Task Force co-chairs.

*"At AEP and Appalachian Power, we're aware of the promise of ICTAS as a transformational entity at Virginia Tech in terms of potential impacts upon energy and sustainability technologies, as well as upon the western Virginia region within which the University is located. The AEP Foundation provides philanthropic support for AEP's and its operating units' goal of supporting and playing an active, positive role in the communities where their employees live and work."*

---R. Daniel Carson, Jr., Vice President

# Thomas Campbell elected member of the Board of Directors of the American Friends of the Alexander von Humboldt Foundation

Thomas Campbell, Ph. D., Associate Director for Special Projects and Outreach and Research Associate Professor with the Institute for Critical Technology and Applied Science (ICTAS), has been elected a member of the Board of Directors of the American Friends of the Alexander von Humboldt Foundation. Campbell joins board members Daniel Fallon, Chair; Ulrike Albrecht, Vice Chair; A. Stephen Dahms, Treasurer; Matthias Vorwerk, Secretary; Thomas Hesse; Eric Koenig; Peggy Kuo; Jaan Laane; Gale Mattox; Arnim Meyburg; and Cathleen Fisher, Ex-Officio Member. The mission of the American Friends is to promote networking, exchange, and creative collaboration among scientists, scholars, artists, and other professionals in the United States and Germany, consistent with the goals of the Alexander von Humboldt Foundation.

Alexander von Humboldt (1769-1859) was a nature researcher and explorer, universal genius and cosmopolitan, scientist and patron. His lengthy Latin American journey from 1799 to 1804 was celebrated as the second scientific discovery of South America. Members of natural science disciplines such as physical geography, climatology, ecology or oceanography see Humboldt as their founder. The masterpiece of his advanced years, the five-volume "Cosmos-

Draft of a Physical Description of the World," has remained unique in its

comprehensive approach.

The "Alexander von Humboldt-Stiftung für Naturforschung und Reisen" (Alexander von Humboldt Foundation for Nature Research and Travel) was established in Berlin 18 months after the death of Alexander von Humboldt in 1860. Until it lost its endowment capital in the inflation of 1923, it essentially provided support for German scientists setting off on research journeys to other countries. A new Alexander von Humboldt Foundation was established by the German Reich in 1925. Its main purpose was now to support foreign students and later academics and doctoral candidates during their stay in Germany. In 1945, the Foundation ceased functioning. Today's Alexander von Humboldt Foundation was established by the Federal Republic of Germany on 10 December 1953, partly at the behest of former Humboldt guest researchers. The headquarters were located then as now in Bonn-Bad Godesberg. Every year, the Alexander von Humboldt Foundation enables more than 2,000 researchers from all over the world to spend time researching in Germany. The Foundation maintains a network of more than 24,000 Humboldtians from all disciplines in over 130 countries worldwide - including 43 Nobel Prize winners.

Campbell's first assignment as a board member was as a guest at the 20th anniversary celebration for the German Chancellor Fellowship held in Washington, D.C. on April 24th. On May 11th, Campbell will attend the first of three yearly board meetings - two to be held in Washington, D.C. and one to be held in Berlin, Germany.



The inaugural **ICTAS Research Day** is planned for September 28, 2010. Keynote speakers will headline activities including building tours, research thrust presentations and a poster session and competition. This event will be by invitation only. For additional information, please contact Thomas Campbell at 540-231-8359 or email: [tomca@vt.edu](mailto:tomca@vt.edu) or Leslie Thornton-O'Brien at 540-231-5244 or email: [lthornto@vt.edu](mailto:lthornto@vt.edu).

*Thomas Campbell*

## 2010 Doctoral Scholars

Eight exceptional Ph.D. candidates, representing five colleges and eight departments, are selected as the Institute for Critical Technology and Applied Science (ICTAS) Doctoral Scholars beginning in the fall semester 2010. This class of eight scholars brings the total of participants currently in the ICTAS program to 34. This program is a collaborative effort supported jointly by departments, colleges, ICTAS and the Graduate School.

The 2010 ICTAS Doctoral Scholars are:

### College of Engineering

Daniel Vanden Berge, Civil and Environmental Engineering  
Konstantinos Krommydas, Computer Science

### College of Science

James Dale, Geosciences  
Chennan Hu, Physics

### College of Agriculture and Life Sciences

Sarah Williams, Plant Pathology and Weed Science  
C. Nathan Jones, Biological Systems Engineering

### College of Natural Resources

Jung Ki Hong, Wood Science and Forest Products

### College of Veterinary Medicine

Daniel Youngstrom, Biomedical and Veterinary Sciences



## ICTAS celebrates the first graduate of the ICTAS Doctoral Scholar Program



Remillieux

ICTAS is proud to announce and share in the celebration of the award of a Ph.D. to Marcel Remillieux, the first graduate of the ICTAS Doctoral Scholar Program. Marcel entered the doctoral program in the department of Mechanical Engineering in the fall semester of 2007 as one of the first eleven participants in the ICTAS Doctoral Scholar Program. Although Marcel had several employment offers to consider upon graduation, he plans to remain at Virginia Tech to complete the scientific work that he initiated during his graduate studies.

"ICTAS is an extraordinary place for being exposed to many cutting-edge fields of science. It was through ICTAS I found out that meaning does not lie beneath things but in between them, this precious interaction from which the mind may open up and creativity may be born," Remillieux explained. "If not for ICTAS I would have missed out on the interaction gained through ICTAS bringing some of the brightest minds the world has to offer in contact with one another."



# ICTAS Awards 2010

The Institute for Critical Technology and Applied Science held an open competition during early 2010 for awards to seed new interdisciplinary research. The initial call requested white paper concept submission, limited to 600 words. Nearly one hundred white papers were reviewed and evaluated. A brief proposal and presentation followed for more than 30 successful white paper submissions.

The competition brought forward many new ideas in the categories of Junior and Emerging Research. ICTAS is pleased to announce that thirteen (13) proposals are selected to receive support beginning July 1, 2010.

Chris Cornelius, Associate Director for Research, ICTAS, said “the funding of these efforts is integral to fostering interdisciplinary research early-stage concept. Additionally, the support of internal advancement of basic concept development is expected to enhance potential for external funding to further develop the ideas, leading to continuing research and exploration in the future.”

The proposals selected for award follow (in alphabetical order by title):

## **Contactless-AC-Modulated Insulator-Based Dielectrophoresis (CiDEP) for Rare Cancer Cell Separation**

Masoud Agah, Electrical and Computer Engineering; Rafael Davalos, School of Biomedical Engineering and Sciences; Eva Schmelz, Human Nutrition, Foods and Exercise.

## **Design and Fabrication of a Biologically Accurate, Vascularized Artificial Bone Graft**

Joseph W. Freeman, School of Biomedical Engineering and Sciences; Aaron Goldstein, Chemical Engineering.

## **Dynamic Mechanical Properties of Recombinant Elastomeric Proteins**

Daniel M. Dudek, Engineering Science and Mechanics; Chenming (Mike) Zhang, Biological Systems Engineering.

## **Hemocompatibility of Drug-laden Nanomaterials**

Elankumaran Subbiah, Center for Molecular Medicine and Infectious Diseases; Nammalwar Sriranganathan, Biomedical Sciences and Pathobiology; Judy Riffle, Chemistry.

## **Hierarchical Design and Assembly of Structures: Nano to Mesoscale**

Amrinder S. Nain, Mechanical Engineering and School of Biomedical Engineering and Sciences; Chris Cornelius, Chemical Engineering; Bahareh Behkam, Mechanical Engineering.

## **Interdisciplinary Teaming and Graduate Education Study of ICTAS**

Maura Borrego, Engineering Education; Roseanne Foti, Psychology.

## **Molecular Target of Soy Genistein for Potential Therapeutic Intervention of Inflammatory Induced Vascular Dysfunction**

Zhenquan Jia, Division of Biomedical Sciences, Virginia College of Osteopathic Medicine; Hara P. Misra, Virginia College of Osteopathic Medicine; Dongmin Liu, Human Nutrition, Foods and Exercise; S. Ansar Ahmed, Biomedical Sciences and Pathobiology.

## **Nanofibers from Multi-layer Melt Electrospinning (MME)**

Eugene G. Joseph, Chemical Engineering; Abby W. Morgan, Chemical Engineering; J. Randy Heflin, Physics.

## **Nanostructure III-V Multijunction Solar Cell on Germanium and Lattice Engineered Silicon Substrates**

Mantu K. Hudait, Electrical and Computer Engineering

## **Novel Electrode Design to Increase Power Generation in Microbial Fuel Cells**

Bahareh Behkam, Mechanical Engineering and School of Biomedical Engineering and Sciences; Michael W. Ellis, Mechanical Engineering.

## **Real-world Oriented Design for Dynamic Spectrum Access Systems**

Yaling Yang, Electrical and Computer Engineering; George Morgan, Finance; Dilip Shome, Finance; Tamal Bose, Electrical and Computer Engineering.

## **The Origin of Nanoscale-derived Properties in Nanoparticles**

M. Murayama, Nanoscale Characterization and Fabrication Laboratory (ICTAS) and Chemical Engineering; William T. Reynolds, Materials Science and Engineering.

## **Using Nanomaterials to Track Messenger RNA in Plants**

James Westwood, Plant Pathology, Physiology and Weed Science; Giti Khodaparast, Physics.

The Institute for Critical Technology and Applied Science at Virginia Polytechnic Institute and State University is an interdisciplinary research institute devoted to investigation in the physical sciences, engineering, biological, behavioral, computation and cognitive sciences.

For more information, please visit <http://www.ictas.vt.edu/index.shtml> or contact Ann Craig at 540-231-2059 or email: [annc@vt.edu](mailto:annc@vt.edu).



Friday, January 29: "Revisiting an Old Puzzle with New Eyes (or, Electron Microscopy of an Incommensurate Structure)"  
with **Bill Reynolds**,  
Director, ICTAS Nanoscale Characterization and Fabrication Laboratory and Professor, Materials Science and Engineering Department, Virginia Tech



Tuesday, February 16: "Beyond Silos: Integrating Interdisciplinary Research and Education in the Academe"  
with **Roop Mahajan**,  
ICTAS Director and James S. Tucker Professor of Engineering, Virginia Tech



Thursday, February 18: "Trimetallic Nitride Endohedral Fullerenes: The Fullerene-based Acceptor component of the Future in OPVs"  
with **Claudia Cardona**,  
Nano/Bio Principal Investigator, Luna nanoWorks, A Division of Luna Innovations Incorporated



Friday, March 12: "μGC Beyond Miniaturizing Gas Chromatography"  
with **Masoud Agah**,  
Assistant Professor, The Bradley Department of Electrical and Computer Engineering, Virginia Tech



Monday, April 5: "A Decade of Sustainable Water Infrastructure Development at the University of North Carolina at Chapel Hill: Successes and Challenges"  
with **Carolyn Elfland**,  
Associate Vice Chancellor for Campus Services, University of North Carolina at Chapel Hill



Friday, April 9: "Investigation of Silicon and Shape Memory Polymer Microactuators for Deployment in Biological Media"  
with **Hrishikesh Panchawagh**,  
MEMS Research Scientist at Eastman Kodak Company, Rochester, NY



Monday, April 12: "Mass Production of Photovoltaic Modules"  
with **W. S. Sampath**,  
Director, Materials Engineering Lab and Associate Professor, Colorado State University



Thursday, April 15: "Text Data Mining applied to Literature Searching, Ethics, Hypothesis Generation, Drug Discovery, Decision Support"  
with **Harold R. "Skip" Garner**,  
Executive Director of the Virginia Bioinformatics Institute, Virginia Tech



Thursday, April 29: "Widespread Adoption of Renewable Energy: Challenges and Material Science Opportunities"  
with **Jeffrey Nelson**,  
Senior Manager, Materials Group, Sandia National Laboratories

## ICTAS Seminar Series

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](mailto:annc@vt.edu).



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Please send comments and address corrections to Ann Craig, [annc@vt.edu](mailto:annc@vt.edu).

Ann Craig, editor | Alex Parrish, graphic designer

## A Different Kind of Seminar Series

In the NY Times best seller, “The Black Swan”, the author (Nassim Nicholas Taleb) defines a Black Swan as an event that has three characteristics: it is an outlier; it carries an extreme impact; it has retrospective predictability. He further makes a claim that our world is dominated by Black Swans. He cites the example of the three recently implemented technologies that most impact our world today-- the Internet, the computer, and the laser -- and notes that all three were unplanned, unpredicted, and unappreciated upon their discovery, and remained unappreciated well after initial use.

While it may not be possible to predict the next Black Swan, it is the contention of ICTAS Director, Roop Mahajan, that we can create an environment and a breeding ground for future Black Swans - an environment in which engineers, scientists and humanists from different disciplines can come together to move beyond the predictable and incremental advances in the current technologies to the disruptive technologies of the future. To this end, the Institute for Critical Technology and Applied Science (ICTAS) is launching a new seminar series entitled “The Black Swan and Disruptive Technology.”

The first seminar of the series, held April 30 in the ICTAS Café X, was introduced by Mark G. McNamee, Senior Vice President and Provost. Roop Mahajan, ICTAS Director and James L. Tucker Professor of Engineering, briefly discussed his vision and the framework of the series and start a dialogue triggered by the question; “What technology/ innovation/idea will make your field irrelevant in seven years?”

Professor Jeff Reed, Willis G. Worcester Professor in ECE and Director of Wireless at Virginia Tech, led a discussion exploring the field of wireless technology in the context of this question.

The second Black Swan Seminar is scheduled for June 25 from 2-4 pm in Café X, ICTAS Building on Stanger Street, Virginia Tech.

