FOCUS ON ENERGY

- Greener Coal-fired Power Plants
- Ionic Liquids for Absorption Refrigeration
- Advanced Nuclear Energy Systems
- Cleaner Radioactive Waste
- More Efficient Wastewater Treatment
- Nano Architecture for Solar Cells
Researchers from each of the five departments within the college are actively addressing energy related issues, such as energy efficiency, safe nuclear waste storage, clean coal utilization, carbon dioxide (CO₂) separation and storage, and renewable energy. Shown above, left to right, are the Environmental Biotechnology Laboratory, the Notre Dame Energy Center, and the Bio/Geo Chemistry Laboratory ... a few of the many facilities in the college focused on energy.

On the cover: Faculty in the College of Engineering employ molecular simulations to investigate the interfacial properties of ionic liquids for a variety of uses, including CO₂ capture and sequestration.

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Dear Friends and Colleagues,

I am pleased to apprise you of some of the outstanding accomplishments in the College of Engineering at the University of Notre Dame this past year. We have established a new record in research awards for the past fiscal year that will surpass $75 million. These awards include a new Energy Frontier Research Center focused on actinide materials, a renewal of our grant in the genomics of malaria, a recently announced ARPA-E grant, and many other significant research awards consistent with the University’s mission to be a “force for good” in the world.

Our faculty have been recognized with a number of national awards this year, including the E. O. Lawrence Award from the Department of Energy for Joan F. Brennecke, the AIAA Aerodynamics Award and recognition as AIAA Fellow for Thomas C. Corke, admission to the National Academy of Engineering and the Indian Academy of Engineering for Ahsan Kareem, and, most recently, the Theophilus Redwood Award from the Royal Society of Chemistry for Paul W. Bohn. The recognition these faculty have received reflects their commitment to excellence and is a harbinger of the kind of impact our faculty will routinely make on applied science and engineering in the coming years.

As we close out this first decade of the century, the College of Engineering is making significant progress in becoming a preeminent research organization. Many of our laboratories and research centers recently moved into the new Stinson-Remick Hall of Engineering, including the Center for Nano Science and Technology, nanofabrication facilities, and the Midwest Institute for Nanoelectronics Discovery. First-year students and graduating seniors have also been taking advantage of the new McCourtney Engineering Learning Center for their many projects.

We have added more than 40 new tenure-track and research faculty to our ranks in the past three years, and we have doubled the level of our research awards. We anticipate additional faculty awards, like those mentioned above, in recognition of faculty members who are involved in foundational research in a variety of areas, including energy, biomedical devices and implants, wireless communications, and environmental issues. This issue of Amplitude, our research publication, will apprise you of some of our recent accomplishments in energy and related areas. We are pleased to share it with you as we dream big for the coming year.

Sincerely,

Peter Kilpatrick
Matthew H. McCloskey Dean of Engineering
Cleaning Coal Emissions

Globally, coal is a cheap and plentiful resource. It fuels more than 40 percent of the electricity worldwide and remains a major player in the energy industry. However, coal-fired power plants emit climate-altering greenhouse gases into the environment daily. To minimize the amount of carbon dioxide (CO₂) released from coal-fired power plants, researchers at Notre Dame are developing ionic liquids that can effectively and economically separate CO₂ from flue gases, so it can be stored underground instead of being released into the atmosphere.

According to Edward J. Maginn, professor of chemical and biomolecular engineering and associate dean for academic programs in the Graduate School, for every pound of coal burned, roughly three pounds of CO₂ is produced. The gases coming out of a coal-fired power plant’s smoke stack contain approximately 15 percent CO₂. The problem is that it has been an expensive proposition to try to capture the CO₂ before it enters the atmosphere.

Current separation technology is an energy-intensive process, taking more than 30 percent of the energy produced to capture the CO₂. In short, a plant has to burn more coal to produce the same amount of "clean" energy. The goal of Maginn’s team is to design a separation process that is more effective and less expensive. They are using computational simulations to design new molecules that can serve as solvents for CO₂. Working with ionic liquids (ILs), salts that are liquid at room temperature, the team can tailor specific properties
of an IL so that it grabs the CO$_2$ and chemically binds to it. Then, as the separation continues, the CO$_2$ flows with the liquid to a high-temperature chamber, where it is released and diverted to a high-pressure pipeline for storage underground, while the benign gases — steam and nitrogen — are released into the atmosphere.

“Because this is such an important issue,” says Maginn, “there are many groups around the world working on a number of different approaches. We were one of the first to begin working with ionic liquids years ago, and we have been fortunate to have several excellent partners in this particular project.” The Notre Dame team consists of four different research groups on campus (led by Maginn, Joan F. Brennecke, Mark McCready, and William Schneider, all faculty in the Department of Chemical and Biomolecular Engineering) and works with Trimeric Corporation, who provides the complex simulations that model the performance of the team’s ILs in an actual power plant. The team also partners with EMD Chemicals Inc., a division of Merck KGaA, who will be making large-scale quantities of the Notre Dame ILs for a pilot test in a large-scale system. The Babcock and Wilcox Company and DTE Energy will also play important roles once the ILs have been refined and are ready for a slipstream run.

To date the team has created several ILs and filed invention disclosures on each of them. They are installing a test unit in the Notre Dame Energy Center in 2011 to run bench-scale tests on the ILs they have developed. Over the next three years, they expect to run large-scale tests in a pilot plant.

“The complex nature of the simulations, and the computational power required to run them, have made the difference in this fundamental research,” says Maginn, “allowing us to make some tremendous strides that would not have been possible even a few years ago.”

**SUGGESTED READING**


Giving 20th-century Absorption Refrigeration Systems the Cold Shoulder

Ideal for carbon dioxide capture, ionic liquids (ILs) — organic salts that are liquid at room temperature — are proving equally as attractive in a variety of energy related applications, including absorption refrigeration. In fact, faculty in the College of Engineering have successfully designed several ILs with specific thermodynamic properties that promise to increase the efficiency of absorption refrigeration systems, providing more cooling for less energy.

Absorption refrigeration, typically used for industrial climate control, is not a new process. Invented in 1858, it replaces the large amounts of electrical energy needed for compressors in normal vapor compression refrigeration units with an energy-stingy pump and low-grade waste heat. Most of today’s systems use an ammonia-water or a water-lithium bromide solution for the refrigerant-absorbent. Both types of systems present challenges.

Much more popular before freons were introduced, ammonia is a toxic compound with a pungent odor. The water-lithium bromide system has other problems: using water as the refrigerant limits the temperature range. If it falls below 32 degrees Fahrenheit, it could form ice in the system, bursting the pipes. Excessive concentrations of lithium bromide, which is a corrosive, can also solidify in the pipes of a system, sending maintenance costs soaring. Neither method is ideal.

Joan F. Brennecke, the Keating-Crawford Professor of Chemical and Biomolecular Engineering and Director of the Notre Dame Energy Center, has been leading a multidisciplinary faculty team in search of a more energy-efficient absorption refrigeration system. It is one of the many projects focused on energy efficiency being conducted in the energy center.

“We know that ionic liquids (ILs) are incredible solvents. They are salts, so they don’t evaporate to cause

Notre Dame researchers are designing ionic liquids with specific thermodynamic properties to address a variety of energy related needs.
air pollution. But, more important in cases like this, we have had a great deal of success designing ILs with unique properties, so that they function the way we want them to in specific processes. That was one of the major reasons we began investigating using water and ILs as the refrigerant-absorbent combination.”

Funded by the Department of Energy, the researchers have been measuring the thermodynamics, including vapor-liquid equilibrium, enthalpy of mixing, and heat capacities, involved in the absorption refrigeration process to calculate the coefficient of performance (COP) for several of the new ILs they have designed. And, they have been very pleased with the results.

The COP for a refrigeration cycle is the cooling that you get divided by the work (power) needed to obtain it. For refrigeration, it is the electrical work needed to run the pump plus the heat you need to add to the absorbent to desorb the refrigerant. A COP of 1.2 or greater is desired for heating efficiency, while 0.7 or greater is the target for cooling.

The next step for Notre Dame will be to build a benchtop model and demonstrate the physical behaviors promised in the simulations. “We’re excited to move to the demonstration phase for stationary systems [making more efficient buildings],” says Brennecke, “but we are equally encouraged about what this work means for mobile cooling systems such as cars and recreational vehicles.”

SUGGESTED READING


Ficke, Lindsay, E.; Rodriguez, Hector; and Brennecke, Joan F., “Heat Capacities and Excess Enthalpies of 1-Ethyl-3-methylimidazolium-based Ionic Liquids and Water,” Journal of Chemical Engineering Data, 2008, 53 (9), 2112-2119.
Laying the Foundation for Cleaner Nuclear Energy

Many people are asking if better materials can be designed for the safe, permanent disposal of nuclear waste? Perhaps the question that should be addressed is not “How can society safely store the dangerous radioactive waste generated by nuclear power plants?” but “Can much of the radioactive waste be recycled into useful fuel, so that storage is less of an issue?” This is one of the basic questions that faculty in the Center for Materials Science of Actinides, a national Energy Frontier Research Center, have been actively pursuing. More specifically, they are seeking ways to control the behavior of uranium and other actinides at the nano-scale to achieve greener and more efficient nuclear energy.

All matter is composed of building blocks. The structures and shapes are different depending on the intended purpose and the materials being used. Uranium, the heaviest abundant element, is the current fuel used in almost all commercial nuclear reactors, but the nuclear waste produced is environmentally troubling. Peter C. Burns, the Massman Professor of Civil Engineering and Geological Sciences and Director of the Center for Materials Science of Actinides, and a team of University researchers have been focusing their efforts on uranium-based building blocks, specifically uranyl peroxide polyoxometalates, to provide a foundation of knowledge for a future advanced nuclear energy system.

Centuries old, polyoxometalates are metal oxide clusters. They are often studied as a model for nano-structured materials and are useful as catalysts in several chemical systems. The structures that Burns’ team is

![Uranyl peroxide self-assembles into clusters with fullerene and other topologies that may be useful in the development of greener nuclear fuel cycles.](image-url)
creating are important because they hold promise for being able to change the behavior of uranium and other actinides used in the nuclear fuel recycling system. They could also be used to manufacture new nuclear fuels with nano-scale precision.

Actinides, such as uranium and neptunium, are ideal candidates for self-assembly into polyoxometalates. In fact, many of the clusters the Burns’ group has discovered exhibit fullerene topologies, meaning they are cage structures that feature 12 pentagons and an even number of hexagons. It is the structure of the cage and, most important, its symmetry that appears to determine the behavior of these clusters. Uranyl peroxide clusters can self-assemble in aqueous solutions. They can be maintained in the solution for several months, and they readily crystallize into extended structures that permit detailed structure characterization. Control of uranium behavior in water by cluster formation may be used to significantly reduce the amount of waste that will actually need to be stored, i.e., a greener fuel cycle that produces more energy without a proportional increase in waste production.

**SUGGESTED READING**


Sigmon, Ginger; Ling, Jie; Unruh, Daniel K.; Moore-Shay, Laura; Ward, Matthew; Weaver, Brittany; and Burns, Peter C., “Uranyl-Peroxide Interactions Favor Nanocluster Self-assembly” *Journal of the American Chemical Society*, 2009, 131 (46), 16648-16649.


Forbes, Tori Z.; McAlpin, J. Gregory; Murphy, Rachel; and Burns, Peter C., “Metal-oxygen Isopolyhedra Assembled into Fullerene Topologies” *Angewandte Chemie International Edition*, 2008, 47, 2824-2827.
Taking the Bite out of Nuclear Waste

The fears surrounding the use of nuclear power are often as highly charged as the spent nuclear fuel produced. During heated discussions, people sometimes forget that nuclear power neither uses fossil fuels nor produces climate-altering emissions. They choose to focus on incidents like “Chernobyl” or “Three Mile Island” instead, while others voice their concerns about the cost of storing nuclear waste and the possibilities of it leaking out of containers and into the environment. All legitimate concerns, these worries need not be show-stoppers on the road to cleaner energy and a carbon-lean or carbon neutral energy portfolio. Researchers at Notre Dame believe they can change the energy picture and satisfy all sides of the nuclear power discussion by better separating the radioactive elements from other materials in the spent fuel.

As of January 2010, there were 436 nuclear power plants operating in 30 countries. Another 56 plants are under construction: China is building nine, Korea six, and India five. The United States is building one.

Many countries generate more of their power from nuclear plants than does the U.S. For example, approximately 77 percent of France’s electricity comes from nuclear power. Lithuania generates 65 percent of its power from nuclear sources, and the U.S. ... 20 percent.

One major drawback, and perhaps the reason that only 15 percent of the world’s power is generated by nuclear plants, has been that once nuclear fuel is spent, it has to be properly stored.

There’s the rub. A nuclear plant can generate 20 metric tons of spent fuel every year. When multiplied by 436 power plants, that’s a lot of radioactive waste that needs to be contained until it decays to safe radioactive levels (hundreds if not thousands of years, according to the U.S. Environmental Protection Agency). The waste also needs to be monitored and guarded. All of this adds to the cost of nuclear energy.

While studying the physico-chemical properties of several actinide borates, Massman Chair Thomas E. Albrecht-Schmitt.

A general view of the NDTB-1 structure, a framework of channels and cages, is shown here. The channels form a network that pierces the whole structure, allowing facile anionic and molecular transport for exchange processes.
**Albrecht-Schmitt** and his team discovered an unusual thorium borate compound (NDTB-1) that can be tailored to absorb ions, including radioactive ions, which could make storage less dangerous and less expensive.

Traditionally, clay has been the material of choice for removing radioactive ions from spent fuel, but clay also removes less harmful ions, like nitrates. And, all of the waste (of high and low-level radioactivity) is then stored together, adding to the cost.

The NDTB-1 grains Albrecht-Schmitt has developed feature eight sides and billions of tiny pores, each with a positive charge that soaks up the negative (harmful) ions in spent nuclear fuel. In fact, the positive electrical charge makes the thorium perfect for this application. It was the only element that offered positively charged pores. To create the thorium grains, the team heated a combination of thorium and boric acid. After the mixture hardened, they immersed it in water to dissolve the excess boric acid, leaving the thorium crystals behind.

The NDTB-1 crystals only remove ions suspended in liquids. Once removed however, the thorium cubes could be added to a solid, storing the most radioactive components of nuclear fission together.

Albrecht-Schmitt’s team has conducted successful laboratory studies using thorium borate crystals, during which they removed approximately 70 percent of the technetium, a highly-radioactive material, from their sample fuel. By changing the size, shape, and charges of the cubes, the team expects to be able to remove as much as 90 percent of the radioactive ions. Field tests conducted at the Savannah River National Laboratory in Aiken, S.C., have shown that NDTB-1 successfully removes technetium from nuclear waste (comparable to waste found at the Hanford site in Washington state).

According to Albrecht-Schmitt, thorium, which is about three times more abundant than uranium, also offers potential as a next-generation nuclear fuel in new reactors, because it would run cleaner and with less waste than uranium-based reactors.

**SUGGESTED READING**


Next-generation Solar Cells: Greater than the Sum of Their Parts

Since the 1950s silicon based solar panels have been used across a multitude of applications. Yet, the production of solar energy is not a mature industry. In the United States alone, it represents a miniscule amount of the total energy generated — less than one percent. Notre Dame researchers, who have already shown that nanoparticles can be tuned to more efficiently harvest energy from the full spectrum of light, are continuing their efforts. Most recently, they have been employing nano-architecture in solar cells that combine two different materials, which operate more efficiently together than when used separately.

Even ten years ago, silicon-based solar cells were not what they are today. They were twice as thick, offered much lower efficiency rates, and had shorter life cycles. It almost cost more energy to manufacture a solar cell than what the cell could generate in its lifetime. Technology has progressed, and today most photovoltaics last 20 to 30 years. The newer thin-film technologies (still silicon based) have lower energy conversion efficiencies, but they offer shorter energy payback times than the first generation of cells.

Professor Prashant V. Kamat and his team have taken another step closer to the next generation of solar cells. They have paired cadmium selenide (CdSe) quantum dots with carbon nanocups (a single-wall carbon nanotube) to show how combining two nano-architectures could offer dramatic improvements in solar cell efficiency and manufacturing cost.

Commercial solar cells are the highest grade photovoltaics on the market today. Since they are made with silicon, they share many of the processing and manufacturing challenges as other semiconductors, including quality control issues and the need for high-vacuum facilities.
“Our cells,” says Kamat, “can be constructed on the benchtop, in a laboratory environment, with purely chemical approaches. The cost is minimal compared to other manufacturing methods.”

Working on the molecular level allows the Notre Dame team to select the light absorption properties, tuning the dots to specific wavelengths of light. For example, metal chalcogenides like CdSe have small bandgaps, so they absorb light in the visible region well. This allows more light to be captured. “What CdSe does not do quite as well as other semiconductor materials,” says Kamat, “is move the captured electrons toward an electrode, where the light can then be converted to energy.” Using only CdSe quantum dots, the electrons take much longer to migrate, wasting much of the potential energy.

To address this, Kamat’s group has paired the CdSe quantum dots with a “stacked cup” carbon nanotube (the nanostructure is arranged like a stack of plastic cups with the bottom cut out). The stack works like a wire to help move the captured electrons along. Although the efficiencies are still not what he thinks they can achieve, Kamat believes each step his team takes brings them closer to developing the next-generation cell. “Between the pace of discovery and the opportunity to explore various combinations with tunable carbon nanostructures, it is an exciting time to be working in this area.”

SUGGESTED READING


More Efficient Wastewater Treatment with Less Energy

Wastewater treatment is essential to protecting human health and the environment, but because of the burgeoning global population, and the increasing need to reuse wastewater, treatment plants are being required to meet even more stringent standards. Most plants will need upgrades to comply with these new regulations. Not only do the changes mean significant capital investments, higher chemical costs, and the production of more greenhouse gases, but they also signal increased energy requirements. A Notre Dame team has developed a novel water treatment technology that helps existing plants meet the new standards using less space, less energy, and less capital, while producing fewer emissions. Equally important, this technology may be adapted to convert a full-sized wastewater treatment plant from an energy sink into an energy source.

Wastewater treatment plants discharge enormous volumes of water, exceeding 100 million gallons of water per day in some larger cities. Although the treatment process varies depending upon the sophistication and age of a plant, it requires a tremendous amount of energy, mainly to aerate the chambers and pump the water.

Conventional wastewater treatment systems use approximately three percent of all of the electrical energy produced in the United States. With the new regulations for nitrogen and phosphorus removal, the process will become even more of an energy drain. It will require larger facilities and more chemicals, making the process more expensive. Greater amounts of greenhouse gases will also be produced as a result of meeting the new standards.

Associate Professor Robert Nerenberg and his team of researchers may have a solution. They have developed a process that reduces the energy requirements for a treatment plant by up to 50 percent while minimizing emissions of nitrous oxide (N₂O), a potent greenhouse gas. The Hybrid Membrane-Biofilm Process (HMBP) they have designed features air-filled hollow-
fiber membranes, which are incorporated into a plant’s activated sludge tank. Once in the tank, a nitrifying biofilm develops on the membranes, producing nitrite and nitrate. By suppressing bulk aeration (instead of supplying it), the liquid becomes anoxic, and the nitrite/nitrate can be reduced with influent bio-chemical oxygen demand (BOD).

Its hybrid nature is what distinguishes the HMBP from other membrane-aerated processes. Heterotrophic bacteria are kept in suspension by maintaining low bulk liquid BOD concentrations, while nitrifying bacteria form a biofilm on the fiber, getting their oxygen by passive diffusion through the air-filled fibers. Thus, the HMBP can save up to 50 percent of the electrical energy required to run the plant, while preventing N₂O emissions and reducing the need for additional chemical additives. Another major advantage is the ability to retrofit existing infrastructure, rather than expand it or replace it with new systems.

After a successful bench-scale study, the team built a pilot reactor, which was tested at the 26th Ward Water Pollution Control Plant in Brooklyn in conjunction with New York’s Applied Research Facility. The pilot study confirmed the ability of the HMBP to achieve total nitrogen removal from an actual wastewater treatment plant in scalable concentrations. Ongoing research, funded by the National Science Foundation, will provide a more basic understanding of the unique microbial processes used in the HMBP.

According to Nerenberg, with a few tweaks the HMBP can also function like a microbial fuel cell, so that in addition to removing the nitrogen and other impurities from the water, it could convert the chemical energy contained in biodegradable compounds into electrical energy. This could allow wastewater treatment plants to send electrical power back to the grid.

**SUGGESTED READING**


Wireless Institute Established at Notre Dame

From one of the first successful wireless transmissions in the United States (sent by Professor Jerome Green in 1899 from the Notre Dame campus to neighboring Saint Mary’s College) to its current research—in areas such as mesh and ad hoc networks, software-defined radio, dynamic spectrum access, wireless sensor networks, and signal detection—the University has a long history of expertise in communications technologies. Building on that history and the substantial achievements of its faculty, the College of Engineering has established the Wireless Institute. According to McCloskey Dean of Engineering Peter Kilpatrick, formation of the institute allows the college to leverage its extensive experience in telecommunications and the Internet as it continues to tackle important interdisciplinary issues that affect society.

J. Nicholas Laneman, associate professor of electrical engineering, will serve as director of the new institute, which engages faculty from the departments of electrical engineering, computer science and engineering, sociology, and finance. A total of 12 faculty, more than 35 graduate students and post-doctoral researchers, and two technical and administrative staff share $2 million in annual research funding, 4,000 square feet of laboratory space, and $4 million in laboratory equipment. “One could argue that wireless technologies are relatively mature, having gone through four or five major surges since the days of Green and other communications pioneers,” says Laneman. “But the pervasiveness of cellular telephony and the mobile Internet are leading to unprecedented opportunities for studying the economic, social, and regulatory aspects of widespread wireless usage, as well as the significant demand for creating new technologies that make more efficient use of the radio spectrum.”

This is the challenge: The radio spectrum is under tremendous pressure to support the exponential growth of mobile users, applications, and data rates. In addition, the process of developing new technologies that enable more efficient use of the radio spectrum, and reallocating spectrum from legacy technologies and services to new ones, is extremely complex.

Signaling formats are different for cellular voice and data, radio and television broadcasting, wireless routers for computer networks, and other wireless technologies. However, each format requires access to radio frequencies to enable valuable services for end users. The growing demand for commercial wireless is requiring regulating agencies such as the Federal Communications Commission to evaluate the merits of various wireless technologies and services in order to decide how to allocate (or reallocate) spectrum going forward. What is certain, given the nature of the issues involved, is that the next surge of innovations will require collaborative efforts by a number of scholars in a variety of areas, like those in the Wireless Institute.

For more information on research and collaborative opportunities in the Wireless Institute, visit wireless.nd.edu.
New Faculty Faces: Recent Hires

Please join the College of Engineering in welcoming its three most recent hires: M. Brian Blake, Harindra Joseph S. Fernando, and Gregory Timp.

Blake, most recently department chair and director of graduate studies in computer science at Georgetown University, has joined the college as associate dean for strategic initiatives and professor of computer science and engineering. An expert in the areas of software engineering, Web services, e-commerce, and related services, Blake will continue his research and teaching activities in service-oriented computing, agents, and workflow technologies; enterprise integration and electronic commerce; software process and life cycles; and software engineering and the Internet.

His administrative responsibilities in the Office of the Dean include the development of faculty and graduate student recruitment and diversity strategies, as well as interaction with corporate and foundation partners on external initiatives.

Fernando, the Wayne and Diana Murdy Professor of Civil Engineering and Geological Sciences, is an expert in fluid mechanics, specifically in atmospheric and oceanic flows, as well as industrial flows involving density variations. His projects include laboratory experiments and field observations in conjunction with theoretical and computer modeling of urban flows, highlighting the effects of climate change; air flow in mountainous terrain; underwater waves in shelf seas; dynamics and remote sensing of ship and submarine wakes; storage problems in National Petroleum Reserves; flow through nuclear reactors; modeling and measurements of air pollution, including health effects; turbulence in the atmospheric boundary layer; and freeway acoustics. He joins the college from Arizona State University, where he most recently served as the director of the Center for Environmental Fluid Dynamics and professor in the Department of Mechanical and Aerospace Engineering, with an appointment in the School of Sustainability.

The first joint appointment between the College of Engineering and the College of Science, Timp’s position is indicative not only of the interdisciplinary nature of his work, but it also signifies the start of a new University program in synthetic biology, which is part of the biomedical initiative on campus. The program seeks to mimic biology on the nanometer scale with man-made constructs for applications in tissue engineering, epigenetics, and DNA sequencing, and will be featured within the University’s Advanced Diagnostics and Therapeutics Initiative.

A recognized authority on nanotechnology, Timp produces everything from nanometer-scale transistors with world-record performance to synthetic nanopores for sequencing DNA. Specifically, he assembles genetically programmed bacteria that act like biochemical signal transmitters, receivers, and logic gates, using a combination of microfluidics, which function like capillaries conveying the cells to an assembly area. He uses arrays of optical tweezers to precisely organize the programmed cells with nanometer-scale precision into a simple computer. Timp came to Notre Dame from the University of Illinois at Urbana-Champaign.

Maginn Receives CoMSEF Early Career Award

Edward J. Maginn, professor of chemical and biomolecular engineering, was named the recipient of the inaugural American Institute of Chemical Engineers Computational Molecular Science and Engineering Forum (CoMSEF) award for outstanding research. He was cited for his “development of algorithms to use molecular simulation to study fundamental thermodynamics and transport behavior and his specific contributions to the understanding of nanoporous materials and ionic liquids.”

A member of the Notre Dame faculty since 1995, Maginn’s research focuses on computational statistical thermodynamics, in which atomistic-level computational methods are developed and utilized to obtain a fundamental understanding of the link between the physical properties of materials and their chemical constitution. Much of his work is devoted to environmental and energy-related applications. He holds two patents and is the author or co-author of more than 80 peer-reviewed articles and five book chapters. He is also on the editorial board of Fluid Phase Equilibria and serves as associate dean for academic programs for the University’s Graduate School.
Robert Nerenberg, associate professor of civil engineering and geological sciences, has been named a 2010 National Science Foundation Early Career Development (CAREER) Award recipient. The CAREER award is the highest honor given by the U.S. government to young faculty in engineering and science.

Nerenberg’s CAREER project, titled “Dynamic Structure and Function of Biofilms for Wastewater Treatment,” uses a novel research platform combining microsensors — bacteria tagged with an anaerobic fluorescent protein — and confocal laser scanning microscopy, to determine the dynamic behavior of bacterial biofilms. The new platform will be used to study the effects of biofilm detachment and re-growth, as well as sudden shifts in nutrient concentrations, on the biofilm microbial community structure, activity, and nitrous oxide (N₂O) emissions. This research is directly relevant to biofilms in wastewater treatment but may also enable research on industrial and clinical biofilms.

Several educational components were included in his proposal. For example, Nerenberg will work with Hispanic students in local schools, encouraging them to pursue careers in engineering and science. He is well suited for this task, given his 14 years living in Argentina, where he obtained his secondary and undergraduate education. He also will train local high school teachers to use simple molecular tools and help them develop teaching modules for their students. In addition, a pilot undergraduate research exchange program with the Pontificia Universidad Católica in Chile will be initiated as a means to provide collaborative international research experiences for undergraduate and graduate students.

Notre Dame and Boeing Enter Research Agreement

The University of Notre Dame and the Boeing Company have entered into a Master Sponsored Research Agreement whereby Boeing funds research projects at the University with a focus on technology translation. The first of its kind under Boeing’s recently implemented enterprise-wide research strategy, the agreement recognizes the University as a premier provider of applied research in aero-optics and flow control. Boeing engineers and researchers and Notre Dame faculty in these disciplines have been collaborating under a number of Air Force contracts and other projects for several years. This agreement provides a framework by which they will continue to collaborate on research of interest to both organizations. Boeing will identify which research projects have the potential to translate to performance improvements of Boeing products and will work jointly with Notre Dame faculty and research engineers in the execution of the research. According to Robert Bernhard, vice president of research at the University and professor of aerospace and mechanical engineering, “We have a long-term, very successful relationship with Boeing and believe the execution of this master agreement provides additional opportunities for our faculty and graduate students to work in close collaboration with one of the truly premier aerospace companies.”

Chawla Joins Health Discovery Corporation Science Advisory Board

Nitesh V. Chawla, assistant professor of computer science and engineering and co-director of the Interdisciplinary Center for Network Science and Applications, has joined the Health Discovery Corporation’s science advisory board.

A faculty member since 2004, Chawla has authored or co-authored more than 90 papers, and his work has been cited more than 1,400 times. His research interests are in the areas of data mining, machine learning, applications of data mining/machine learning, distributed computing for data mining/machine learning, pattern recognition, biometrics, bioinformatics, intelligent scientific visualization, and customer analytics.

Health Discovery Corporation is a molecular diagnostics company that uses advanced mathematical techniques to analyze large amounts of data to uncover otherwise undetectable patterns. Its primary business focuses on licensing its intellectual property and developing its own product line of biomarker based diagnostic tests.

Nerenberg Receives CAREER Award

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A faculty member since 2004, Nerenberg’s research centers on biofilm processes in environmental engineering, especially for water and wastewater treatment. He and his team have developed a novel wastewater treatment process, the Hybrid Membrane-Biofilm Process, that reduces energy requirements by up to 50 percent and minimizes emissions of N₂O (see page 12).
Robert Moran Professor of Civil Engineering and Geological Sciences Ahsan Kareem has been elected a foreign fellow of the Indian National Academy of Engineering. With this election, he joins an elite group of engineers from India who are also leaders in the United States. Kareem, who is director of the NatHaz Modeling Laboratory, has long been involved in research and educational initiatives in India, including his work at the Structural Engineering Research Center in Chennai (Madras) as a United Nations Development Program consultant. In collaboration with the researchers there, he has been developing a major cyclone resistant design initiative using the large-scale facilities in the center.

Earlier this year Kareem was also elected a member of the U.S. National Academy of Engineering (NAE), one of the highest professional distinctions accorded to an engineer who has made outstanding contributions to engineering research, practice, or education.

Most recently, he was elected by the American Society of Civil Engineers (ASCE) as a distinguished member. Distinguished members are those individuals whose contributions to civil engineering are legendary, as are their leadership and research.

A Notre Dame faculty member since 1990, Kareem specializes in probabilistic structural dynamics, fluid-structure interactions, structural safety, the mitigation of natural hazards and applications of cyberinfrastructure for the analysis and design of civil infrastructure. In addition, he has served in the administration, management, and organization of numerous professional societies, including the ASCE, as well as committees of the National Research Council, NAS/NAE, the International Association for Wind Engineering, and the American Association for Wind Engineering.

Kareem Honored by Indian Academy, NAE, and ASCE

Clark Equipment Professor of Aerospace and Mechanical Engineering Thomas C. Corke has been named a fellow of the American Institute of Aeronautics and Astronautics (AIAA). According to the institute, AIAA fellows are “persons of distinction who have made notable and valuable contributions to the arts, sciences or technology of aeronautics or astronautics.” The award was presented at the AIAA Fellows Dinner in Arlington, Va., on May 11.

He was also recently selected by the AIAA to receive the 2010 Aerodynamics Award. This award is presented annually in recognition of meritorious achievement in the field of applied aerodynamics and notable contributions in the development application, and evaluation of aerodynamic concepts and methods. Corke was cited for his “strong commitment to academic and research achievement, consistent record of superior technical accomplishment and numerous experimental and computational contributions to aerodynamics.” A bronze medal and certificate will be presented to him during the AIAA Awards Luncheon during the Applied Aerodynamics Conference in Chicago this summer.

The founding director of Notre Dame’s Institute for Flow Physics and Control and director of the Hessert Laboratory for Aerospace Research, Corke specializes in the study of fluid mechanics. His research interests are in the area of fluid mechanics, specifically related to hydrodynamic stability, transition of laminar flow to turbulent flow, aeroacoustics, computational fluid dynamics, applied turbulence control, unsteady flows, wind engineering and atmospheric diffusion, and wind tunnel design.

A faculty member since 1999, Corke is a fellow of the American Physical Society and the American Society of Mechanical Engineers. His research on plasmas has been emulated worldwide for flow control applications and includes a new type of plasma sensor designed for use in hypersonic Mach number, high enthalpy flows. He also is the author of “Design of Aircraft,” which has been adopted as the capstone design text in more than a dozen aerospace departments across the United States and in numerous programs around the world.

Corke Honored by AIAA: Named Fellow and Aerodynamics Award Recipient
A distinguished panel of 41 planetary experts from Europe, the United States, Mexico, Canada, and Japan that included Clive R. Neal, professor of civil and geological sciences, has determined that fossil evidence clearly indicates a mass extinction event occurred on Earth approximately 65.5 million years ago, ending the Age of the Dinosaurs. The event, known as the Chicxulub Impact because of the 1991 discovery of a 200-kilometer wide meteorite crater in the Yucatán province of Mexico, has been used by geologists to define the end of the Cretaceous period and beginning of the Paleogene period. In a paper published in the March 5, 2010, issue of Science, Neal and the team of experts detailed their analysis of the data taken from the sulfate-rich sediments of the Chicxulub crater. Specifically, Neal examined geochemical changes across the time of the extinctions, called the K-Pg boundary, as well as the influence of volcanic activity in India about the same time. The team believes that further studies of the crater, integrated climate models, and fossil records will reveal additional information about the physical and biological mechanisms involved not only in the K-Pg mass extinction but other extinction events in Earth history.

A faculty member since 1990, Neal’s studies are not limited to the Earth and its environment. His interests include the evolution of the moon and Mars, as well as the origin of the solar system. In fact, as chair of NASA’s Lunar Exploration Analysis Group — which is responsible for analyzing scientific, technical, commercial, and operational issues associated with lunar exploration, Neal was recently briefed on the LCROSS lunar-impact probe mission.

LCROSS, an empty-stage rocket, was sent crashing into the moon on Oct. 9 while a trailing satellite measured the dust and chemicals from the impact. In November NASA announced that the probe found significant quantities of water in the crash plume. The mission confirmed that information found at the Apollo sites were not representative of the entire moon, while also supporting the results found by the Moon Mineralogy Mapper instrument on the Indian Chandrayaan-1, which found water on the lunar surface outside the permanently shadowed regions of the moon.

According to Neal, who is also a member of NASA’s Lunar Science Institute (LSI), the results demonstrate that there are resources available on the moon that could support human return to the moon to establish a permanent habitat. The LSI is a select team of scientists tasked with growing the nation’s technical capabilities in lunar science and developing educational opportunities in space science.

Planetary Geologist Makes His Own Impact

Kirk A. Reinbold has been named managing director of the Advanced Diagnostics and Therapeutics (AD&T) Initiative. The AD&T designs micro-sensing devices for personalized health care and environmental monitoring. Researchers within the AD&T are developing miniaturized systems that can capture and detect a few distinct molecules in order to provide physicians and scientists with more accurate information for medical diagnoses or environmental assessments.

In this newly created position, Reinbold serves as the chief operating officer of the AD&T and is responsible for managing the activities of the initiative, including the development of relationships with foundations, government agencies, and university and commercial partners, including large companies and start-up ventures. He also oversees complex multi-investigator proposals from development through funding dispersal, as well as the activities of 24 principal investigators, numerous other researchers, and support staff.

Reinbold, who holds several patents for inventions related to neurological impairment rehabilitation, osteoarthritis management, and sports performance monitoring, previously served on the Scientific Advisory Board of a telehealth company that develops at-home monitoring systems. He also served as senior consultant and medical science liaison for MedTech Solutions.

AD&T Names Managing Director
One of the challenges to improving the country’s technological preeminence is the education of qualified students ... not only to engineering and scientific principles but also to the innovation process. The 2009-10 academic year ushered in an inaugural group of 29 students pursuing a master’s of science degree in engineering, science, technology, and entrepreneurship at Notre Dame. The new Engineering, Science, and Technology Entrepreneurship Excellence Master’s (ESTEEM) program represents the collaboration of the College of Science, the College of Engineering, and the Mendoza College of Business. Its purpose is to prepare an elite group of recent graduates in the fields of engineering, science, and mathematics for a future where they will lead technological advances.

ESTEEM students are learning valuable skills to help them transform the technical engineering and scientific skills they already possess into commercially viable products and processes with societal and economic value. In addition to coursework focused on finance, technical marketing, operations management, and R&D management, each student is required to complete a capstone business plan for a high-tech start-up company. Current student projects range from tissue vaccines and nanotechnology-based solar cells to passive smart windows and the optimum design of structures for crashworthiness. At the end of the 12-month program, each student will be fully capable of starting his or her own small company or creating new opportunities in larger corporations.

In addition to faculty guidance, the students are able to take advantage of the facilities in the newly opened Innovation Park at Notre Dame, a business incubator designed to facilitate the migration of research and new venture ideas into the marketplace. The collaborative space offered at Innovation Park encourages students to interact with the executives of companies also located in the facility. They are able to observe and participate in the process of technology transfer from concept to end-user, including technology development and validation, business plan fundamentals, financial processes, manufacturing, and marketing.

Laser-based communications offer advantages over other methods for point-to-point contact: They are faster, lighter, less expensive, and more secure. In January 2010, a team of researchers led by Eric Jumper, professor of aerospace and mechanical engineering, successfully completed the first in a series of in-flight tests on the aero-optic wave front sensor system developed at the University. These initial flight tests helped ensure the performance of the system in flight, to determine that the software can overcome aircraft vibration. Over the next two years an additional series of formation flights will help test different optical configurations that can be used to mitigate the effects of turbulence on the laser energy exiting the aircraft through a system turret.

The configurations involve vortex generators and fairings on the outside of the aircraft and electronic methods called “adaptive optics” on the inside. Once the team completes the formation flights, the Air Force will conduct additional system tests on larger aircraft. (The preliminary tests conducted by Notre Dame will save the Air Force millions of dollars.)

If it can be perfected, the wideband laser communications links enabled through the Notre Dame system would bolster the success of reconnaissance vehicles. For example, the system could be used for disaster relief in places like Haiti, providing better real-time pictures of the location of refugees and helping determine the best method or route to deliver needed supplies. The systems could also be used for communications between aircraft, between an aircraft and the ground or a satellite or to provide high-speed Internet service during a commercial airline flight.
Jay B. Brockman, associate dean for educational programs and associate professor of computer science and engineering, was one of only 49 engineering researchers and educators who participated in the National Academy of Engineering’s first Frontiers of Engineering Education symposium. During the symposium, these young faculty members shared ideas regarding best practices and research in engineering education and explore innovations to help them build a stronger infrastructure for 21st-century engineering education.

Brockman, who joined the Notre Dame faculty in 1992, oversees college-wide educational initiatives. He also solicits federal and industrial funding to support innovative educational opportunities for engineering students. He recently published “Introduction to Engineering: Modeling and Problem Solving,” which helps students understand the world of engineering and career options. The book’s goal, like that of the University’s first-year engineering course sequence, is to facilitate the successful transition of students from thinking like high school students to thinking like engineers.

Brockman’s research interests also include the design of digital systems and integrated circuits, computer architecture, high-performance computing, multidisciplinary design optimization, and engineering education, especially the bridge between high school and college.

Associate Professor James Schmiedeler was one of the 88 outstanding young engineers selected to take part in the National Academy of Engineering’s 15th annual U.S. Frontiers of Engineering Symposium in September 2009. During the symposium, the participants — engineers from academia, industry, and government ages 30 to 45 who have been recognized for their exceptional engineering and technical work in a variety of disciplines — examined engineering tools for scientific discovery, the health care delivery system, new applications for nano- and micro-photonics, and resilient and sustainable infrastructure.

A Notre Dame graduate, Schmiedeler returned to the University as a faculty member in the Department of Aerospace and Mechanical Engineering in 2008. He had previously served as an assistant professor at The Ohio State University.

Schmiedeler’s research interests encompass the areas of kinematics, dynamics, and machine design, particularly as applied to the development of robotic systems, and an understanding of human motor coordination. His current work focuses on biped robot locomotion, human recovery from stroke and spinal cord injury, robot-assisted rehabilitation, and human impact injury biomechanics.

Joan F. Brennecke, the Keating-Crawford Professor of Chemical and Biomolecular Engineering and Director of the Notre Dame Energy Center, was selected to receive the 2009 Ernest Orlando Lawrence Award from the U.S. Department of Energy (DOE). The Lawrence Award honors engineers and scientists at mid-career for their exceptional contributions in research and development supporting the DOE and its mission to advance the national, economic, and energy security of the country. It is given in each of the following areas: chemistry, materials research, environmental science and technology, life sciences, nuclear technologies, national security, and non-proliferation and high energy and nuclear physics.

Recognized for “her seminal work advancing fundamental understanding in supercritical fluids and ionic liquids, and her scientific and technological leadership in discovering new environmentally-benign, green chemistries,” Brennecke (and the other honorees) received a citation signed by the Secretary of the DOE, gold medal, and honorarium in a ceremony earlier this year.

A faculty member since 1989, Brennecke has received numerous awards for her research, as well as her contributions in the classroom, including the 2008 Julius Stieglitz Lecturer Award from the American Chemical Society, the 2007 John M. Prausnitz Award from the Conference on Properties and Phase Equilibria for Product and Process Design, and the Professional Progress Award from the American Institute of Chemical Engineers.

Schmiedeler Selected for Frontiers of Engineering

Brennecke Receives Lawrence Award

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Brockman Participates in Engineering Education Symposium
One-of-a-Kind Programming Course Targets Microsoft® Surface™

According to Aaron Striegel, associate professor of computer science and engineering, College of Engineering undergraduates are taking advantage of the one-of-a-kind programming course he has been teaching using the Microsoft® Surface™. A multi-touch computer that responds to human movement and objects placed upon it, the Microsoft Surface helps people interact with the digital world in a simple and intuitive way. One of the applications students have developed during the course is called SurfaceBand. Inspired by popular games such as RockBand™ and Guitar Hero®, players test their ability to hit musical notes [eye-hand coordination] as they scroll across the screen. While the students learn how to program the Surface, faculty have been working with it in another way.

According to the American Heart Association, stroke is the No. 3 killer in the United States. It is also a leading cause of long-term disabilities, particularly motor deficiencies in arm movement. An interdisciplinary team led by Striegel, James Schmiedeler, associate professor of aerospace and mechanical engineering, and Charles Crowell, associate professor of psychology, is working to extend the capabilities of “game” devices such as the Nintendo® Wii™ and multi-touch devices like the Surface to enhance rehabilitation activities after a stroke or traumatic injury. They have partnered with Johan Kuitse, the director of Rehabilitation Services, and his staff at Memorial Hospital in South Bend.

Although the Surface has received limited attention for rehabilitation (by virtue of its games), the team is exploring novel applications. They are also working to identify how the devices can be used to better diagnose motor and cognitive impairments, to quantifiably measure the recovery of motor and cognitive function, and to speed and enhance that recovery in stroke rehabilitation patients.
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