

College of Engineering  
*2012 Annual Report*

Chemical Engineering

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Message from the department head



The chemical engineering department at Kansas State University is committed to improving student training; strengthening its research capabilities; providing effective public service; and promoting stronger local, national and international recognition of the program.

As detailed in this report, renovation of our research laboratories was the department’s most significant milestone in 2012. This made the laboratories safer and more energy efficient, while enabling new types of research. As part of the renovation, graduate students were moved to newly furnished offices in Seaton Hall. By grouping all students together, they are better informed about all of the department’s research, and this has led to greater interactions between students.

The decade-long increase in the size of the department continues. From 2003 to 2012, the number of undergraduates in the department increased from 104 to 233. International students are a significant part of this increase; currently, they comprise 15% of the undergraduates in the department. The number of Ph.D. candidates is also increasing, from a five-year average of 11 (2002-2006) to 19 (2008-2012).

The department is benefiting from the University Engineering Initiative Act (UEIA), which will fund new scholarships, a new engineering building (phase four to the engineering complex), and faculty and staff positions. This 10-year (2013-2023) program was established by the Kansas State Legislature to increase the number of graduates with B.S degrees in engineering. This investment has been motivated by the recognition that engineers create new jobs and contribute to economic growth in Kansas.

To enhance its reputation and to advance student learning, the department’s faculty members and students publish papers based on their research, and give presentations at professional meetings and at other universities. We host graduate seminar speakers from government labs and other universities to learn about cutting-edge research and to show them our department; they are always impressed by the variety and depth of K-State research. The department is also advanced by faculty members regularly serving on national proposal review panels and editorial boards. Starting in 2012, John Schlup began serving as a program evaluator for ABET. Furthermore, the department’s external advisory board has become increasingly active in promoting the department by improving publicity about the department, establishing funds to recognize faculty contributions (as well as retaining competent faculty) and ensuring the undergraduate curriculum is relevant to industry.

The university recognizes the experience and expertise of the department’s faculty. Mary Rezac led the K-State 2025 Research Task Force to identify the university’s strengths and opportunities for investment that can bring it greater recognition. Keith Hohn served on the K-State 2025 Undergraduate Research Task Force, the goal of which was to define, assess, and improve undergraduate research opportunities and quality.

The hard work of our faculty, staff and students, in addition to support from the administration and our alumni, indicates a bright future for the department. I am indeed excited by these prospects.

*James H. Edgar*  
James H. Edgar  
Chemical Engineering Department Head  
Tom H. Barrett Faculty Chair



# Molecular matchmaker:

## Professor develops process, device to aid in sustainable energy practice



as fuel. Instead, the oxygen is removed in a process called hydrotreating, Rezac said. In conventional hydrotreating, pressure is used to force hydrogen into the liquid bio-oil where it chemically reacts and strips away some of the oxygen from the oil, making water as a by-product.

“In this conventional method you need a great deal of hydrogen and the reactor has to be really big,” Rezac said. “There has to be a lot of catalyst for a little bit of oil and it has to be done at very high pressures. Typically it takes 2,000 pounds of pressure per square inch to force the gas down to the catalyst to react with the oxygen.”

The group has been able to reduce the amount of hydrogen and pressure needed by using the membrane to serve as a contact point between the liquid and gas phases. In the membrane contactor, the hydrogen is supplied by diffusion through the membrane while the oil flows past the metal surface. In this way, the hydrogen avoids direct solution in the oil and the subsequent diffusion through it. In the membrane system, the hydrogen is supplied directly to the catalytic site making it readily available for reaction.

“We did an early-stage run with about 30 pounds of pressure per square inch, which is about the same amount of pressure you’d have in your bike tire,” Rezac said. “We’ve demonstrated that we can effectively hydrotreat bio-oil on the small scale. Now we are confirming how to do it on a larger, more continuous scale.”

Once the bio-oil is relieved of its extra oxygen molecules, it is similar to petroleum oil and can go through the same process for final conversion into fuel, Rezac said. The decreased hydrogen dependency should help make the process a more viable option for sustainable energy.

“Hydrogen availability is a very fair concern since we are currently hydrogen poor,” Rezac said. “The membrane is not necessarily going to solve the whole hydrogen deficiency problem — because it’s a big problem — but if we reduce hydrogen demand for this system, then that will make it better.”

As co-director of the university’s Center for Sustainable Energy, Rezac is creating partnerships across the university with scientists, agriculturalists, economists and other engineers to further research on improving sustainable energy practices. One of her roles is to facilitate groups of researchers to work

together to develop solutions for large problems, such as how to produce energy from biomass in a sustainable manner.

Her matchmaking role continues as she helps potential participants appreciate the benefits they’ll receive if they enter the partnership. The center has been successful in developing several projects, including a multimillion dollar, multiyear project with funding from the National Science Foundation to train students in the interdisciplinary problems associated with the production of sustainable bioenergy. More information can be found at [igert.ksu.edu](http://igert.ksu.edu).

Her success in her research would not be possible without the hard work of the many graduate students in her lab. She has mentored more than 30 graduate students who are now employed in a variety of industries from academia to pharmaceutical and petrochemical companies. Training the next generation of chemical engineers is one of her favorite parts of her job.

“I really get excited when my graduate students are successful,” Rezac said. “Maybe more so than when my own research activities are successful, because the impact of what I can do gets multiplied by the successes of the students I work with.”

— K-State Communications and Marketing



Playing the role as a chemical bond matchmaker, Kansas State University’s Mary Rezac, ConocoPhillips professor of sustainable energy and professor of chemical engineering, is improving possibilities for sustainable energy.

Rezac, in collaboration with Peter Pfromm, professor of chemical engineering, and their research groups, is making the conversion of bio-oil to biofuel more efficient by developing membrane contactors. In the new reactor, a membrane, decorated with metal catalyst particles, provides a suitable place for the bio-oil to easily bond with hydrogen.

“Making and breaking chemical bonds is somewhat difficult to do,” Rezac said. “It is easy to write down on paper but it is hard to force the molecules together in a reactor, so we are using membranes to help bring two molecules together.”

The bio-oil is derived from plant material that contains many carbohydrates and has too much oxygen to be used directly



## Durland Hall research laboratories renovated

Research laboratories in Durland Hall were expanded in size and extensively renovated in 2012 to meet current needs of the faculty, and to improve the lab's safety, functionality and energy efficiency. Since Durland Hall's completion in 1976, the chemical engineering department's research activities had evolved, creating the need for new capabilities.

"These newly renovated laboratories improve the analytical and synthesis capabilities of the chemical engineering department and enable new types of research to be investigated," said Jim Edgar, chemical engineering department head. "Students will receive better training and education in these state-of-the-art facilities, and the laboratories will be a valuable resource for K-State students and faculty for many years."

Total cost of the renovation was \$2.6 million. Mary Rezac, chemical engineering professor, was principal investigator on a \$1.6 million grant from the National Science Foundation, through the American Recovery and Reinvestment Act of 2009, which provided base support for the project. Additional funding was provided by corporate and individual donors, the College of Engineering and the university.

To celebrate completion of the renovation, an open house was held Sept. 15, 2012, with approximately 100 students, faculty and alumni attending and touring the laboratories. Guest speakers were K-State President Kurt Schulz, John English, dean of the college of engineering and Edgar.

Changes made to the facilities included the following:

Five large laboratories plus a staging area were created by combining nine laboratories and 10 offices. This resulted in more than 5,000 square feet of renovated laboratories—a 25% expansion.

Safety showers, eye wash stations, overhead sprinklers and exits were updated to meet current safety standards. The laboratories now have true wall-to-ceiling walls which will provide better containment of chemical releases or fires. Entry into the laboratories requires a numerical code, providing better security.

The number of fume hoods was increased from seven to 15. The new units incorporate flow monitors to assure users they are functioning correctly. This also added energy efficiency as sashes automatically close when not in use.

The laboratories were designed to encourage more collaboration between research groups. A central corridor connects three of the laboratories and the staging area, allowing students to easily pass from one lab to another.

Facilities were incorporated to meet specific research demands of K-State researchers. This included the aforementioned fume hoods designed for acid use as well as ventilated cabinets dedicated to storing toxic gases.

Windows between the laboratories and the hall were included to facilitate tours through Durland, better showcasing the department's research.

The renovation allowed consolidation of faculty equipment into one space. A professor's equipment can now all be stored in one laboratory instead of dispersed across five different laboratories as in the past.

The laboratories incorporated a number of modern features such as diffuse, direct and indirect lighting; seamless epoxy floors; adjustable, overhead electrical outlets to eliminate the need for extension cords; individual ventilation and air-conditioning systems; and plenty of storage cabinets.



**NSF grant helps graduate student participate in Japanese summer research experience**

A summer spent in Japan helped a chemical engineering graduate student experience new cultures and approach science with a different perspective.

Clint Frye, doctoral student in chemical engineering, spent 10 weeks in Japan as part of a National Science Foundation East Asia and Pacific Summer Institute grant. The grant included more than \$6,000, a \$5,000 stipend and traveling expenses. Frye was one of 60 recipients for summer 2012. Frye's faculty adviser is James Edgar, professor and head of the department of chemical engineering.

While in Japan, Frye researched thermoelectric material with Takao Mori, a researcher at the National Institute for Materials Science in Tsukuba, Japan. The trip overseas was Frye's first study abroad opportunity.

"The world is getting more globalized and the need for international collaboration is becoming increasingly important," Frye said. "What I found to be truly rewarding is seeing how science is done in an entirely different culture. Coming from an American culture and living as an international student gave me the opportunity to watch other people take a completely different approach to the same research topic that I study. It made me learn a lot about myself."

—K-State Communications and Marketing





# Faculty



**James H. Edgar**

Department Head and Professor  
Tom H. Barrett Faculty Chair

Ph.D., Chemical Engineering, University of Florida, 1987  
B.S., Chemical Engineering, University of Kansas, 1981

Research: Application of chemical engineering to semiconductor processing

Teaching: Engineering materials, thermodynamics, nanotechnology, solid-state devices, unit operations



**Jennifer L. Anthony**

Associate Professor

Ph.D., Chemical Engineering, University of Notre Dame, 2004  
M.S., Chemical Engineering, University of Notre Dame, 2003  
B.S., Chemical Engineering, University of Colorado (Boulder), 1999

Research: Advanced materials, molecular sieves, environmental applications, ionic liquids

Teaching: Thermodynamics, separational process design, transport phenomena laboratory



**Vikas Berry**

Associate Professor

William H. Honstead Professor of Chemical Engineering

Ph.D., Chemical Engineering, Virginia Polytechnic Institute and State University, 2006  
M.S., Chemical Engineering, University of Kansas, 2003  
B.S., Chemical Engineering, Indian Institute of Technology - Delhi, India, 1999

Research: Graphene science, bionanotechnology, materials science, molecular electromechanics, sensors, electronic devices, impermeable coatings

Teaching: Reaction engineering, electronic materials, transport phenomena, basic concepts in material science and engineering, mechanical properties



**Larry Erickson**

Professor

Ph.D., Chemical Engineering, Kansas State University, 1964  
B.S., Chemical Engineering, Kansas State University, 1960

Research: Air quality applications of nanoscale materials to indoor environments, remediation of contaminated soil and groundwater, beneficial effects of vegetation in contaminated soil, sustainable energy

Teaching: Seminars on sustainability, hazardous waste engineering, air quality, process systems design



**L. T. Fan**

University Distinguished Professor

M.S., Mathematics, West Virginia University, 1958  
Ph.D., Chemical Engineering, West Virginia University, 1957  
M.S., Chemical Engineering, Kansas State University, 1954  
B.S., Chemical Engineering, National Taiwan University (Taiwan), 1951

Research: Process systems engineering (including process synthesis and control), biochemical engineering (including biomass hydrolysis and gasification and downstream processing), chemical reaction engineering, particle technology (including fluidization and solids mixing), environmental pollution control

Teaching: Chemical reaction engineering, advanced process design and optimization, chemical engineering analysis



**Larry A. Glasgow**

Professor

Ph.D., Chemical Engineering, University of Missouri, 1977  
M.S., Chemical Engineering, University of Missouri, 1974  
B.S., Chemical Engineering, University of Missouri, 1972

Research: Interaction of turbulence with fluid-borne entities in multi-phase processes; flocculation, aggregate breakage, aggregate deformation, expulsion of interstitial fluid from floc structures and the effects of oscillatory fluid motions upon interphase transport; bubble formation, coalescence and breakage in aerated reactors; effects of energetic interfacial phenomena upon cells in culture; impulsive distribution of small particles in air-filled chambers

Teaching: Chemical process dynamics and control, transport phenomena laboratory, process analysis, chemical engineering analysis



**Keith L. Hohn**

Professor

Ph.D., Chemical Engineering, University of Minnesota, 1999  
B.S., Chemical Engineering, University of Kansas, 1995

Research: Catalysis and reaction engineering, natural gas conversion, hydrogen generation, millisecond contact time reactors, nanoparticle catalysts, chemical and fuels from biomass

Teaching: Unit operations lab, chemical engineering analysis, current topics in chemical engineering, chemical reaction engineering, systems design



**Peter H. Pfromm**

Professor

Ph.D., Chemical Engineering, University of Texas (Austin), 1994  
M.S., Process Engineering, University of Stuttgart (Germany), 1985

Research: Polymers in membrane separations and surface science

Teaching: Computational techniques in chemical engineering, bioseparations, separational process design, biochemical engineering, chemical process dynamics and control



**Mary E. Rezac**

Professor

ConocoPhillips Professor of Sustainability Energy

Ph.D., Chemical Engineering, University of Texas (Austin), 1993  
M.S., Chemical Engineering, University of Texas (Austin), 1992  
B.S., Chemical Engineering, Kansas State University, 1987

Research: Mass transport, polymer science, membrane separation processes, hybrid system (reactor-separator) designs, applications to biological systems, environmental control, novel materials, sustainable energy

Teaching: Mass and energy balances, separation processes, unit operations lab, sustainable energy topics



**John R. Schlup**

Professor

Ph.D., Chemical Engineering, California Institute of Technology, 1981  
B.S., Chemical Engineering, Kansas State University, 1975  
B.S., Chemistry, Kansas State University, 1974

Research: Applied spectroscopy, thermal analysis, intelligent processing of materials, kinetics of polymerization reactions, biobased industrial products

Teaching: Transport phenomena laboratory, systems design, electronic and structural materials, surface phenomena, polymer science



### Membrane Reactor Technology for Combined Reaction and Separations

Biofuels and biobased products can improve environmental quality, rural economies and national security through the cross-disciplinary efforts of scientists and engineers with an appreciation for the complexity of the societal, technological and scientific issues involved. Key to success in this field is efficient reactions and biorefining, the separation of biologically derived, high-value chemicals. Compared to the processing of petrochemical products, bio-based refining technology is still at its infancy. Recent efforts have focused on developing bio-based, specific processing technology. However, the majority of the ongoing research in this field is devoted towards fuels rather than chemicals. The importance of chemicals can be realized from the fact that petrochemicals consume only 3.4% of the crude oil in a refinery but generate revenue roughly equivalent to fuels, which consume 70.6% of the crude oil. To realize a high return on investment, it is imperative for a biorefinery to produce industrially useful chemicals along with fuels.

This research is focused on membrane reactor technology to promote succinic acid hydrogenation at mild operating conditions (1 atm pressure). Asymmetric membranes with a thin, defect-free polymer layer are employed as a contactor between aqueous-phase and gas-phase hydrogen. The skin of the membrane contactor is decorated with metal catalytic sites. The aqueous feed solution is continuously pumped past the catalytic surface and hydrogen is supplied from the permeate side. Characterization of the membrane is performed, as defects in the skin layer and thickness of

this layer play important roles in regulating the supply of hydrogen to the catalyst surface. This research examines the effect of membrane flux, presence of skin-layer defects and catalyst loading on the performance of the membrane reactor system.

Dr. Peter Pfromm  
Dr. Mary E. Rezac

### Solar Processing for Sustainable Production of Ammonia

The production of ammonia, commonly used in agriculture as a fertilizer, consumes several percent of the world's energy budget. Producing a pound of ammonia currently consumes more than a pound of natural gas. The increasing demand for food, along with plans to use more biomass to produce fuels, points towards increasing demand for fertilizers (and thereby ammonia) for many years to come. In addition, the options of using ammonia as a fuel in diesel engines or as a hydrogen carrier for an on-board hydrogen supply for vehicles are currently being investigated elsewhere.

At K-State, the potential of using solar energy to produce ammonia at mild process conditions is being explored. The goal is to create a sustainable production of ammonia based on an inorganic reaction cycle driven by concentrated sunlight. The overall cycle converts water, air and biomass, or another carbon source, into ammonia and valuable syngas. Both ammonia and syngas can be used as an energy carrier or as feedstock for chemical synthesis.

Another approach integrates solar hydrogen production with the ammonia synthesis process with the benefit of converting solar-derived hydrogen to an easily stored and transported form



(ammonia). No carbon source is needed. Ammonia easily exceeds current benchmarks for hydrogen storage approaches set by the U.S. Department of Energy in regard to a hydrogen economy.

This project is supported by the NSF IGERT program "I-STAR BioEnergy" at Kansas State University. Experimental research, process design and economic evaluation are integrated for this project.

Dr. Peter Pfromm  
Dr. Vincent Amanor-Boadu (Agricultural Economics)

### Reducing the Energy Demand of Bio-Ethanol

Ethanol from fermentation processes is produced widely in Brazil, and the U.S. has embarked on a path to reach very significant ethanol production using fermentation. All fermentation-based ethanol production faces the issue of the energy intensive ethanol/water separation following fermentation. This is especially true for cellulosic-based bio-ethanol that produces rather dilute ethanol/water mixtures due to the fermentation parameters.

This project explores use of salt-extractive distillation enabled by a membrane-based salt recycling process to lower the energy demand of the ethanol/water separation. Calcium chloride can greatly improve distillation performance. Electrodialysis is used to recover salt from the distillation process and recycle it. Process simulation, including customized thermodynamics and economic evaluation, is used to integrate the experimental design parameters for the membrane process in the intricate separation network to recover fuel-grade ethanol from the fermentation broth. Significant energy savings will accrue, and this will help to improve the energy balance and sustainability of bioethanol.

Dr. Peter Pfromm

### Economic and Technological Sustainability of Bio-Based Energy Approaches

A multi-disciplinary collaboration between Drs. Amanor-Boadu (agricultural economics), Nelson (resources) and Pfromm (engineering) has resulted in an initial publication on the tech-

nological sustainability of algae-based diesel that has found some resonance. Several publications have already taken note of the work. The second part of this sustainability analysis for algae diesel (economic sustainability interrogated by dynamic stochastic economic evaluation) is in review for publication.

The project team anticipates applying its interdisciplinary approach to sustainability to more processes in the future.

Dr. Peter Pfromm  
Dr. Vincent Amanor-Boadu (Agricultural Economics)  
Dr. Richard Nelson (Center for Sustainable Energy)

### The Role of Ionic Liquids in the Synthesis of Nanoporous Materials

Ionic liquids are organic compounds composed of ions and are liquids near room temperature. They are good alternatives to water as a solvent, in part because of their extremely low vapor pressures. Their specific properties can be tailored by changing their molecular structure, specifically the ligands composing the molecules. Research is focusing on using a combination of solubility and spectroscopy measurements, thermodynamic theory and molecular modeling to study nanoporous materials made via ionothermal synthesis, where the solvent is an ionic liquid. The effect of systematic changes to the ionic liquid structure on the interactions with the nanomaterial precursors and how that in turn affects the formation of the final material is under investigation. This work is developing (1) the first solubility measurements of nanomaterial precursors in ionic liquids, (2) thermodynamic models to describe the phase behavior of the precursors and ionic liquids, (3) crucial validation of molecular dynamics simulations for ionic liquid / precursor systems, (4) quantification of the chemical complexes formed between the solute and solvent in the initial stages of zeolite synthesis, and (5) elucidation of trends between the solute/solvent phase behavior and material formation that will be used to rationally select ionic liquids solvents for synthesis of novel nanoporous materials.

Dr. Jennifer Anthony





# Research highlights

## Transport Studies in Chemical Engineering

Principal interests in this study concern the interaction of turbulence with fluid-borne entities in multi-phase processes. Specific areas of study include flocculation, aggregate breakage, aggregate deformation, expulsion of interstitial fluid from floc structures and effects of oscillatory fluid motions upon interphase transport. In addition, investigation includes bubble formation, coalescence and breakage in aerated reactors, effects of energetic interfacial phenomena upon cells in culture, and impulsive distribution of small particles in air-filled chambers. A study has also been initiated on the effectiveness of a passive mixing device for the treatment of agricultural wastewaters.

Dr. Larry Glasgow

## Applied Spectroscopic and Thermal Analysis Techniques in Material Synthesis

This research project has two emphases: application of spectroscopic and thermal analysis techniques to chemical engineering problems, and use of biorenewable resources as feedstocks for engineering materials. Currently infrared spectroscopic methods are being developed to monitor *in situ* the early stages in the synthesis of mesoporous materials (in collaboration with Dr. Anthony).

Dr. John Schlup

## Heterogeneous Catalysis for Energy Production

Heterogeneous catalysis is important for increasing the efficiency and reducing the cost to produce valuable chemicals. This is especially true for energy production. Three current projects are ongoing in this area in the chemical engineering department at K-State.

In the first project, new catalysts are being developed for con-

verting biomass to fuels and chemicals that are easily separable from feed and product stocks. Magnetic nanoparticles are being acid-functionalized to break down cellulose to fermentable sugars. The nanoparticles offer a number of advantages over other acid catalysts: they are easily separable using a magnet, their acidity can be modified through choice of functional group and they are reusable.

In the second project, a hybrid biochemical/catalytic processes is being developed to produce chemicals from biomass. In this approach, fermentation converts biomass to useful intermediate chemicals (such as 2,3-butanediol), which are then converted to chemicals like methyl ethyl ketone or a liquid fuel-precursor like butene. By using both biochemical and catalytic processes, researchers are harnessing the positive features of each (fermentation can be highly specific to one product, catalytic reactions can be very fast) while minimizing their negative aspects (fermentation can be slow, catalytic reactions are not always selective).

A final research interest is the production of hydrogen from liquid fuels through catalytic partial oxidation. Bimetallic catalysts are being developed to convert military logistic fuels like JP-8 to hydrogen, where it can be used in fuel cells for portable power generation. The bimetallic Pt/Ni catalysts being developed offer a number of advantages: catalyst cost is decreased by replacing some Pt with Ni and the two metals offer complementary features (Pt is very active for oxidation, while Ni is active for steam reforming reactions).

All projects include synthesization of the catalysts, characterization of their physical and chemical properties using a variety of techniques (x-ray photoelectron spectroscopy, infrared spectroscopy, temperature-programmed methods, x-ray diffraction), and testing their catalyst activity for the reaction of interest.

Dr. Keith Hohn

## Crystal Growth and Epitaxy of Boron Compound Semiconductors

Semiconductors are key component in many solid-state devices including diodes and transistors in integrated circuits for computers and cell phones, light-emitting diodes (LEDs) and laser diodes (LDs) for general illumination, information displays, and for DVD and Blu-ray players. Important advantages of solid-state devices are their low-power requirements, speed, low-cost compactness and robust nature (resistance to impact damage).

Three boron compound semiconductors, boron nitride (BN), boron phosphide (BP) and icosahedral boron arsenide ( $B_{12}As_{12}$ ), are being studied at K-State for their potential applications in radiation detection and radioisotope batteries. These semiconductors have properties distinctively different than the most commonly used semiconductors, such as silicon and gallium arsenide. For example, one isotope of boron ( $B-10$ ) reacts strongly with neutrons—much more strongly than most elements. This reaction produces charged particles that are relatively easy to detect, making a solid-state neutron detector possible. Such neutron detectors would find applications in homeland security, medical diagnostics, petroleum exploration and fundamental science. These could provide a low-cost alternative to the most common neutron detectors which rely on helium-3, a particularly scarce and expensive isotope of helium.

Some boron compound semiconductors are extraordinarily resistant to radiation damage. Under intense radiation, the electrical properties of most semiconductors quickly degrade, leading to device failure. In contrast, such failure could be avoided in devices based on icosahedral boron arsenide. An intriguing application of this property is the betacell, a device that directly converts nuclear energy to electrical energy. These devices could take advantage of the enormous energy densities of nuclear energy sources that can be 10,000 times higher than gasoline. Nuclear sources can also provide energy for decades, much longer than chemical batteries.

At K-State, we are focusing on developing synthesis techniques that produce boron compound semiconductors of high crystal perfection and low residual impurity concentrations. Bulk crystals are produced by precipitation from molten metal solutions and thin films are prepared by chemical vapor deposition. The former produces relatively thick crystals with low defect densities, while the latter produces thin films either with low residual impurity concentrations or with intentionally added impurities to tailor the electrical properties. The structural, optical, chemical and electrical properties of these materials are characterized to provide feedback for optimizing the synthesis process. Through further process optimization, the goals are to produce these materials with the quality needed for the novel electronic devices envisioned.

Dr. J. H. Edgar

## High Dielectric Oxides on Nitride Semiconductors

Properties of the semiconductor gallium nitride are favorable for high-power, high-frequency and high-temperature electronics. Applications include power amplifiers for military radar and automobile collision avoidance, base stations for cell phones and hybrid car power electronics. However, designers of its electronic devices have generally avoided using insulating layers, due to the poor electrical properties of the insulator-semiconductor interface. Insulating layers are almost universally found in silicon-based electronic devices, because they enable large voltage swings and greatly reduce leakage currents. These benefits could also be realized with gallium nitride devices, if a technology for preparing a good insulator on semiconductor can be found.

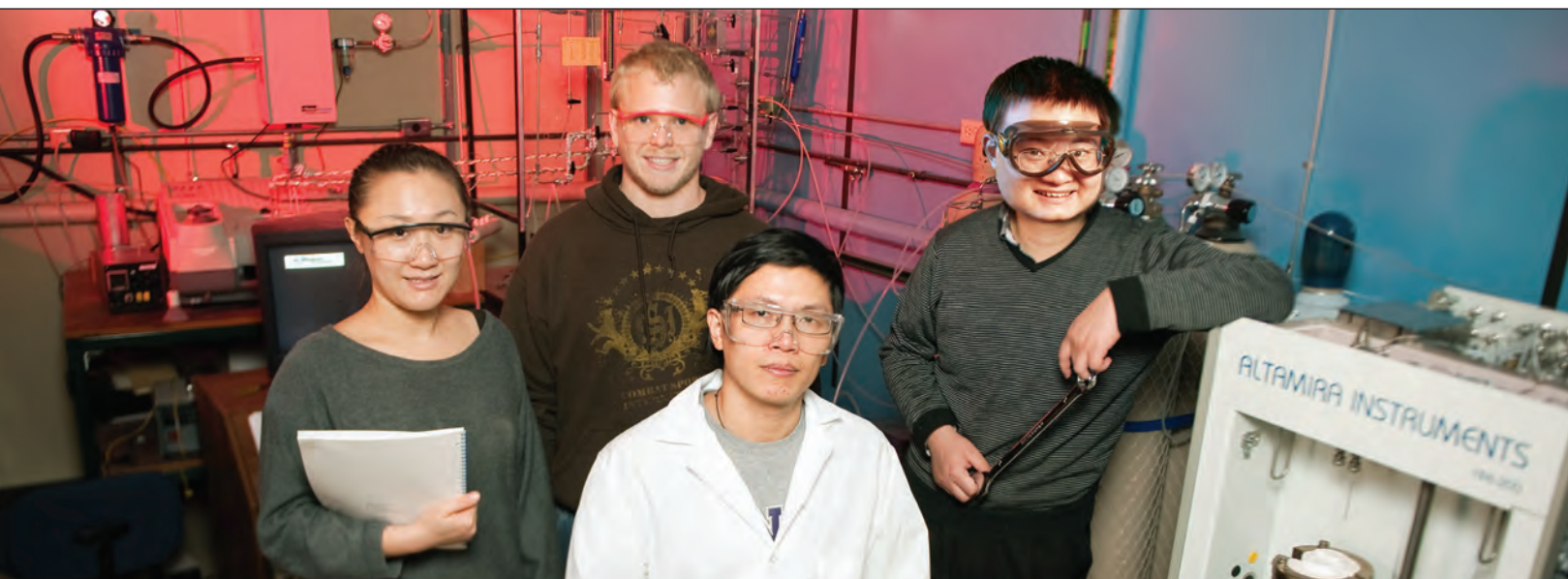
The technology to do this is being developed at K-State with collaborators at the Naval Research Laboratory. Properties of the insulator-gallium nitride interface are being optimized by developing an understanding of how process conditions impact the properties. First, insulators with high dielectric constants, such as alumina ( $Al_2O_3$ ) and titanium dioxide ( $TiO_2$ ), are deposited on GaN by atomic layer deposition. Then the morphology, structure and composition of the oxides are established through detailed characterization. Next, electrical properties are measured, trends are identified, and these are interpreted based on physical and chemical properties. The goal is to establish the most important properties necessary so as to produce high-quality electronic device performance. This technology would greatly improve the versatility of this new semiconductor in power electronics.

Dr. J. H. Edgar

## Graphene and Its Derivatives: Modifications and Applications

Graphene, two-dimensional sheets of carbon a single atom thick, exhibits many unique mechanical, optical and electronic properties that have the potential for many device applications. Recent theories have shown that by controllably manipulating graphene's structure and chemistry, its properties can be tuned over a broad range and new quantum physics can be realized. Synthesis and property characterization studies at K-State include the study of graphene, which was (a) chemically modified with gold nanostructures, (b) functionalized via metal-coordination bonds, (c) nanostructured into quantum dots and nanoribbons, (d) composited with biocompatible polymer to produce bacterial repellent paper, (e) functionalized with a molecular machine and (f) modified into a molecular protein-carpet to wrap bacterial cells for enhanced electron microscopy imaging.

Similar studies are also being applied to hexagonal boron nitride, another material that forms atomically thin two-dimensional sheets. Its properties are distinctly different: while graphene is typically a conductor, boron nitride is an insulator. At K-State, a





novel process was developed to exfoliate boron-nitride atomically thick sheets with the highest yield reported to date. Research to chemically functionalize boron nitride sheets is ongoing.

Recent highlights with graphene include developing (1) true-scale imaging of bacterial cells under an electron microscope by wrapping the cells with impermeable graphene to prevent water loss, (2) a process to produce graphene nanostructures with unprecedented structural control over its length and width dimensions, (3) a process to functionalize graphene while retaining its high-charge carrier mobility (a major current challenge hampering graphene research) and (4) a graphene-based device capable of detecting molecular mechanics.

Dr. Vikas Berry

## Environmental Applications of Chemical Engineering

Chemical engineers have expertise to work on environmental problems related to sustainable energy, environmental management and sustainability. Several research problems are related to air emissions and liquid and solid effluents from industrial and agricultural processes. One current problem is development of a treatment wetland to manage sulfur and other inorganic compounds in flue-gas desulfurization wastewater from a coal-burning power plant. The research involves both mathematical models and experimental work. Faculty and students from four departments are working with a consulting company as a multidisciplinary team. New technology development to address environmental problems and advance sustainability is a second area of research.

Larry E. Erickson



## Mitigating Pollutant and Pathogen Contamination in Livestock Operations

This cooperative project with the biological and agricultural engineering department, sponsored by the K-State Agriculture Experiment Station, aims at comprehensive analysis and optimal synthesis of systems for mitigation of pollutant and pathogen emissions from livestock sources and operations involving wide-ranging activities. Such activities include operation and management of beef cattle feedlots, swine buildings, dairy barns and poultry farms. Expected outcomes of the project will be the optimal systems synthesized, which will provide the definitive framework for the design, operation, control and management of sustainable infrastructures and facilities for reducing and/or eliminating pollutants and pathogens in a variety of livestock operations. The project will be executed as follows.

First, additional processes available for mitigation of pollutant and pathogen emissions from livestock sources and operations will be thoroughly searched and identified, thus augmenting those already generated or collected by the project members. Second, domain knowledge and data pertaining to the characteristics and behavior of the processes identified will be systematically compiled and logically categorized. Moreover, consistency of the data compiled will be statistically assessed within each of the categories established. Third, the processes identified will be modeled based on domain knowledge and data pertaining to them by resorting to deterministic and stochastic approaches. The resultant mechanistic models will be simulated via conventional numerical techniques as well as stochastic simulation methods, e.g., the Monte Carlo method, under a wide range of realistic scenarios. Fourth, the systems' optimal configurations will be determined, i.e., the optimal systems will be synthesized, by incorporating the processes identified and classified at the outset by mainly resorting to the graph-theoretic method based on process graphs (P-graphs). Nevertheless, if the system of interest comprises a small number of functioning units, it can be synthesized via a heuristic or conventional algorithmic method. Fifth, sustainability of the optimal systems synthesized will be assessed in light of various criteria such as cost, energy requirement, exergy consumption, material requirements and environmental impacts. An initial estimation of the sustainability will be performed through the method of sustainability potential; if the resultant potential is deemed favorable, it will be further assessed by one or more of the available methods for the evaluation of sustainability.

Whenever necessary or desirable, some statistically designed laboratory and field experiments will be carried out to generate supplementary data, confirm the results of modeling and simulation, and/or assess the performance of synthesized systems.

L. T. Fan

## Jennifer L. Anthony

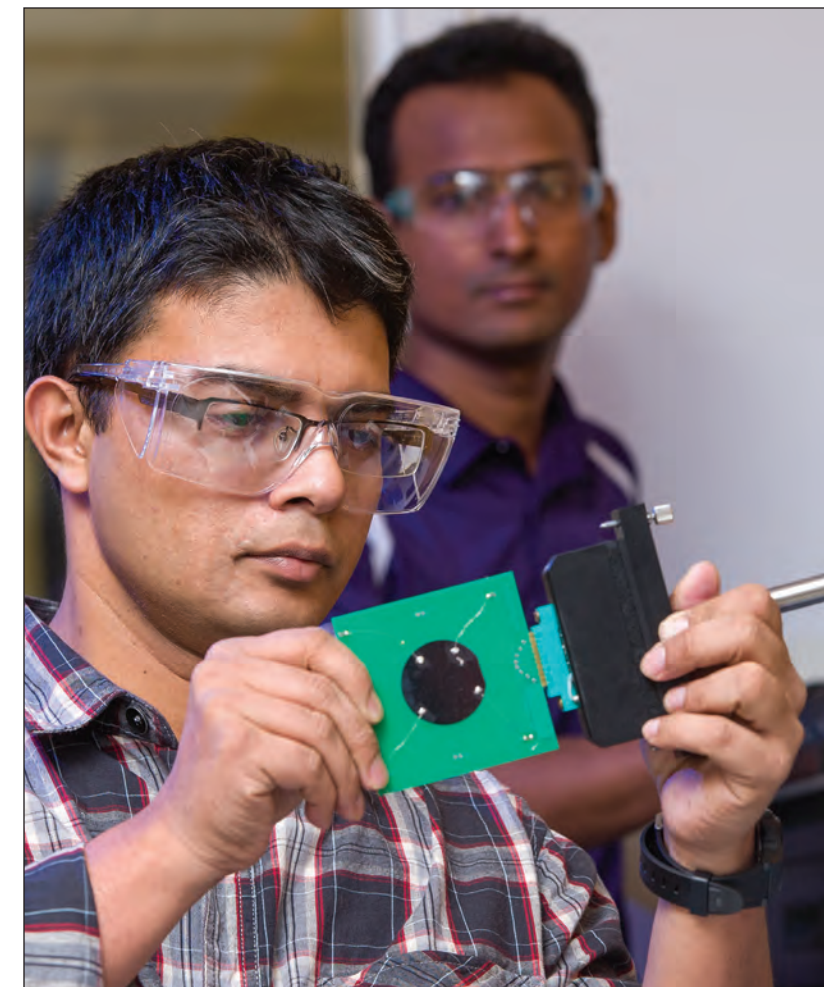
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## Vikas Berry

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## James H. Edgar

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## Larry Erickson

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## L. T. Fan

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## Keith L. Hohn

- Cingarapu, S., D.B. Hamal, M.A. Ikenberry, C.M. Sorensen, K. Hohn, and K.J. Klabunde, "Transformation of Indium Nanoparticles to  $\alpha$ -Indium Sulfide: Digestive Ripening and Visible Light-Induced Photocatalytic Properties," *Langmuir* 28, 3569-3575 (2012).
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## Peter H. Pfromm

- Michalsky, R., P.H. Pfromm, "An Ionicity Rationale to Design Solid-Phase Metal Nitride Reactants for Solar Ammonia Production," *J. Phys. Chem. C*, 116 (44), 23243-2325, 2012.
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- Michalsky, R., P.H. Pfromm, "Thermodynamics of metal reactants for ammonia synthesis from steam, nitrogen and biomass at atmospheric pressure," *AIChE Journal*, 58 (10), 3203-3213, 2012.
- Hussain, M.A.M., J.L. Anthony, P.H. Pfromm, "Reducing the energy demand of corn-based fuel ethanol through salt-extractive distillation enabled by electrodialysis," *AIChE Journal*, 58, 1, 163-172, 2012.

## Jennifer Anthony

- Co-PI, "Synthesis of Nanoporous Zeolitic Materials in Ionic Liquids: A Fundamental Study of the Solvent's Role," Submitted to the National Science Foundation, PIs: Dr. Jennifer L. Anthony and Dr. Timothy I. Morrow (LA Tech). \$274,966 over three years (JLA share: \$249,724) Funding Period: August 2008-July 2011, continued through July 2012.
- PI, "Graduate Research Supplement (GRS) for CBET—0829024—Synthesis of Nanoporous Materials in Ionic Liquids: A Fundamental Study of the Solvent's Role," Submitted to the National Science Foundation, Requested \$41,799 over one year. Funding Period: May 2010-April 2011, continued through July 2012.

## Vikas Berry

- PI, "Tapered Graphene Nanoribbons of Controlled Width and Tapering Angle: Carrier-Tunable Diode Transistor." Office of Naval Research; Amount \$300,000; Start Date: 01/01/11; Period = 3 Years.
- PI, "CAREER: Detailed Characterization of Graphene Quantum Dots of Controlled Size, Shape and Chemistry." NSF; Amount \$400,000; Start Date: 02/01/11; Period = 5 Years.
- PI, "Growth and Transfer of Large-Area Graphene on Silicon and Silica Substrates and Its Surface Engineering." MEMC Inc; Amount \$237,913; Start Date: 04/01/11; Period = 3 Years.
- PI, "Detailed Surface Engineering and Electrical Characterization of  $\pi$ -Functionalized Graphene Sheets and Ribbons with Preserved Lattice and Electronic Characteristics." NSF; Amount \$301,704; Start Date: 08/15/10; Period = 3 Years.
- Co-PI, "MRI: Acquisition of a Field-Emission Scanning Electron Microscope for Kansas State University," PI: James Edgar, Co-PIs: Christopher Sorensen, and Jun Li. NSF; Amount \$518,928; Start Date: 09/01/09; Period = 3 Years.
- PI, "Study of Graphene Nanoribbon's Structural Properties Using STM: Determining Edge-Crystallographic Orientation and Defects." Brookhaven National Laboratory; Equipment Usage Time Granted on STM; Period = 3 Years.

## James H. Edgar

- PI, High-K-Oxide Insulating Gate Group III Nitride-Based FETs, Department of Defense Experimental Program to Stimulate Competitive Research (DEPSCoR), 2010-2013, \$452,710.
- PI, ARI-MA: Collaborative Research: Hexagonal Boron Nitride-Based Neutron Detectors, National Science Founda-

tion, 2010-2015, \$961,788 (KSU portion), with J. Geuther (KSU) and Texas Tech University.

- PI, Materials Development of Boron Phosphide-Based Neutron Detectors, Department of Energy, 2010-2012, \$560,000.
- PI, MRI: Acquisition of a Field-Emission Scanning Electron Microscope for Kansas State University, NSF (lead P.I., with 14 other KSU faculty), 2009-2012, \$725,400 (NSF: \$518,928; KSU:\$206,472).
- Sustainable Energy Solutions via Systems-Based Research: Modernizing the Sustainable Energy Research Infrastructure in Durland Hall, National Science Foundation (M.E. Rezac, Principal Investigator), 2010-2013, \$1,598,997.

## Larry Erickson

- NSF REU "Earth, Wind and Fire: Sustainable Energy for the 21st Century," (with Keith Hohn and others).
- NSF Grant EEC-1156549, "REU Site: Earth, Wind and Fire: Sustainable Energy in the 21st Century," \$99,085 for first year with 3-year duration, March 15, 2012 - February 28, 2015. With Keith Hohn. This is a renewal award.
- NSF EPSCoR "Climate Change and Energy: Basic Science Impacts and Mitigation," K. Bowman James PI with investigators at KU, KSU and WSU.
- EPA "Sustainable Gardening Initiatives at Brownfield Sites," with Ganga Hettiarachchi, Sabine Martin, Blase Leven and others.
- Westar, and Burns and McDonnell, "Westar Wetlands Pilot Project," with Stacy Hutchinson, Ganga Hettiarachchi, and Larry Davis. \$377,524, 2 years.
- Black and Veatch Foundation Grant for \$200,000, "Building a World of Difference with Solar-Powered Charge Stations for Electric Vehicles," \$40,000/year for 5 years with start date of October 24, 2012. Anil Pahwa co-PI. The following are listed in the proposal: M.W. Babcock, T. Boguski, G.L. Brase, W. Griswold, K.L. Hohn, K.W. Kramer, B.A. Leven, R.D. Miller, B. Mirafzal, B. Natarajan, N. Schulz and R. Stokes.

## L. T. Fan

- R.G. Maghirang and L.T. Fan, "Mitigating Pollutant and Pathogen Contamination in Livestock Operations," AES, 10/01/2010-09/30/2015, \$34,867.
- A donation of \$8,000 received from Judi Fan and Robert Reay.

## Keith L. Hohn

- Co-PI (with Larry Erickson), NSF, "REU Site: Earth, Wind and Fire: Sustainable Energy for the 21st Century," \$316,398, 3/12-2/15.





- “Bimetallic Nanoparticle Catalysts for Reforming of Hydrocarbon Fuels” (PI at KSU, with Franklin Kroh at Nanoscale Corporation), DOD STTR Phase II, \$300,000 (KH share), 9/11-8/13.
- Senior personnel (with PIs Jun Li, Judy Wu, and Francis D’Souza), “Nanotechnology for Renewable Energy,” NSF EPSCoR, \$28,000 out of \$800,000 per year, 6/2009-5/2014.
- Senior personnel (with PIs Jun Li, James Edgar, and Christopher Sorensen), “Acquisition of a Field-Emission Scanning Electron Microscope for Kansas State University,” \$518,928, 1/10-1/13.
- Co-PI (with Donghai Wang, BAE), “Acid-Functionalized Nanoparticles for Hydrolysis of Lignocellulosic Biomass,” NSF, \$322,999, 9/10-8/13.
- Co-PI (with Dan Higgins), “Single-Molecule Spectroscopy for Characterization of Mesoporous Acid Catalysts,” ACS-PRF New Directions, \$100, 1/11-12/12.
- Senior personnel (with Mary Rezac, Peter Pfromm, Teresa Selfa, Laszlo Kulcsar, Praveen Vadlani, Krista Walton, Donghai Wang, Wenquia Yuan, Kyle Mankin, Richard Nelson, DeAnn Presley, Charles Rice, Scott Staggenborg), “From Crops to Commuting: Integrating the Social, Technological and Agricultural Aspects of Renewable and Sustainable Biorefining (I-STAR),” NSF IGERT, \$3,199,996, 09/09-06/14.
- “Modeling of NSCR Performance with Exhaust Mixtures from Natural Gas-Fueled Engines,” (PI), Pipeline Research Consortium International, \$53,262, 1/1/12-12/31/12.



## Peter H. Pfromm

- PI (with M.E. Rezac, Co-PIs Pfromm, Mankin, and Peterson), “IGERT: from crops to commuting,” National Science Foundation DGE, 2009-2014, total overall \$3,171,485 from NSF.
- Co-PI (with M. Rezac), “Membrane reactor technology for the efficient conversion of biomass to industrial chemicals,” USDA AFRI, \$587,000, 2010-2013.

## Mary E. Rezac

- IGERT: Integrating the Social, Technological and Agricultural Aspects of Renewable and Sustainable Biorefining (I-STAR), Funded by National Science Foundation Budget: \$3,171,485, Period: September 2009 – August 2014, University Hard-Dollar Match: \$410,000.
- Center for Sustainable Energy Support, Funded by ConocoPhillips, Budget: \$750,000, Period: July 2009 – June 2014.
- Membrane Reactor Evaluation for Specialty Chemicals Production: Phase II, Funded by DOE SBIR Program, Joint with Compact Membrane Systems, KSU Budget: \$190,691, Period: August 2008 – August 2012.
- Center for Sustainable Energy Support, Funded by Department of Energy, Budget: \$1,213,625, Period: October 2009 – October 2012.
- Biobased Products and Bioenergy, Multi-University Graduate Program, Joint with South Dakota State University, University of Arkansas, Oklahoma State University, Funded by USDA, Budget: \$498,290, Period: August 2009 – July 2012.
- Sustainable Energy Solutions via Systems-Based Research: A Proposal to Modernize the Sustainable Energy Research Infrastructure in Durland Hall, Funded by: National Science Foundation, Budget: \$1,598,997, Period: October 2010 – October 2013.
- Membrane Reactor Technology for the Efficient Conversion of Biomass to Industrial Chemicals, Funded by USDA AFRI, Budget: \$586,427, Period: December 2010 – November 2013.
- REU Site: Summer Academy in Sustainable BioEnergy, Funded by National Science Foundation, Budget: \$297,351, Period: March 2011 – April 2014.

## John R. Schlup

- “BNCT Using Novel Method of Stem Cells as Boron Carriers: Synthesis of Boron-Containing Compounds for Attachment to Stem Cells,” John R. Schlup and Jessica Long, Johnson Center for Basic Cancer Research (Kansas State University), 2011 – 2012 academic year, \$1,000. Renewed for 2012 – 2013 academic year.

## Jennifer Anthony

- Most Approachable Professor Award
- Reviewer, manuscripts for various journals
- Adviser, AIChE chapter

## Vikas Berry

- William H. Honstead Endowed Professorship
- Research featured at State of the University address by university president
- Research featured in American Chemical Society videos
- Invited speaker, Materials Research Society and Electrochemical Society meetings
- Editorial board member, Scientific Reports journal
- Advisory board member, Journal of Nanoscience Letters and All Results Journal-Nano

## James H. Edgar

- Tom H. Barrett University Faculty Chair
- Reviewer, manuscripts for numerous journals
- Collaborator, Naval Research Laboratory

## Larry Erickson

- Treasurer, environmental division, AIChE
- Treasurer, chemical engineering and law forum, AIChE
- Editorial board member, Environmental Progress and Sustainable Energy
- Editorial board member, International Journal of Phytoremediation
- Session chair, AIChE annual meeting
- Member, Kansas Natural Resource Council Board
- President, Kansas Natural Resource Council

## L. T. Fan

- Honoree, special issue, Ind. Eng. Chem. Res.
- Member, scientific advising committee, Texas Hazardous Waste Research Center, Lamar University
- Participant, University Distinguished Professors Forum
- Reviewer, various manuscripts for technical journals and miscellaneous research proposals





### Larry A. Glasgow

- Book manuscript in progress, 10 chapters completed (Applied Mathematics for Science and Engineering)
- Reviewer, manuscript for AIChE Journal

### Keith L. Hohn

- James L. Hollis Memorial Award for Excellence in Undergraduate Teaching
- Segebrecht Distinguished Faculty Achievement Award
- Presenter, Kansas EPSCoR conference, NSF EPSCoR KNE meeting, and KSU IGERT Symposium series
- Session co-chair, AIChE national meeting
- Reviewer, numerous journals and proposals
- Editor-in-chief, Catalysts—international, peer-reviewed online journal
- Theme leader, biofuels research, NSF EPSCoR project
- Member, three NSF review panels

### Peter H. Pfromm

- Reviewer, various peer-reviewed journals and government agencies

### Mary E. Rezac

- Senior Award for greatest inspiration to the senior class
- Chair, 2025 Strategic Planning Committee on Strategic Research Themes

### John R. Schlup

- Participant, 3rd North American Materials Education Symposium
- Presenter, A Seven-Trait Writing Tool for Assessment of Technical Writing, ABET Symposium
- PEV, AIChE and ABET accreditation visit to a chemical engineering department

### Distinctive characteristics of the chemical engineering graduate program at Kansas State University include the following:

#### ■ Emphasis on educating Ph.D. students

Since 2007, the department has admitted primarily Ph.D. candidates to increase its research productivity, thereby enhancing its recognition among peer institutes. The ratio of Ph.D. to M.S. candidates is approximately 10:1.

#### ■ Strong financial support for graduate students

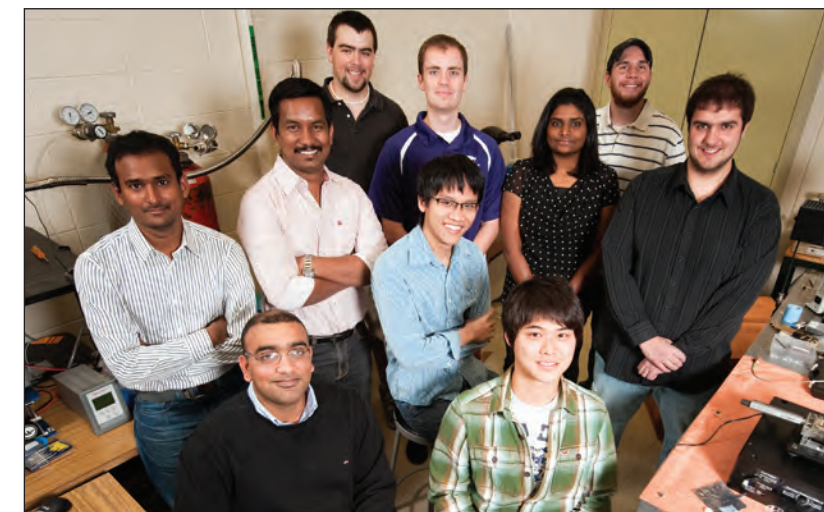
All on-campus students receive competitive stipends in addition to their tuition. The department is, therefore, selective in accepting the highest quality, most committed applicants to the graduate program. This solid financial support makes it possible for students to focus on their studies and research. Funding comes from industrial contracts or donations, government grants and private gifts.

#### ■ Extensive multidisciplinary collaborations

Faculty and graduate students collaborate with a wide variety of other disciplines and institutions (both universities and government laboratories) to access needed expertise for their projects. Most of the papers from the department involved co-authors from other disciplines and institutions. Collaborators included faculty and researchers from countries such as Hungary, the Netherlands, Germany, the UK and Poland; and from disciplines such as chemistry, biochemistry, grain science, materials science and engineering, mechanical engineering and computer science. These collaborative efforts are tremendously beneficial to students' educational experience by providing wide-ranging perspectives.

#### ■ Excellent educational and professional development opportunities for students

Classes taken by students comprise a combination of advance core chemical engineering courses in thermodynamics, reaction engineering, transport phenomena and process systems engineering that develop depth; and electives courses in mathematics, sciences and engineering fields that enable students to acquire expertise in their specialties. Through research, students learn new analytical and experimental skills by practice, strategies for problem solving and the ability to work independently as well as collaboratively. Students learn effective oral and written communication through presentations at professional meetings and publications in technical journals. They also work closely with their advisers and collaborators, learning from their experiences and expertise. This frequently involves traveling to attend meetings or to visit government laboratories and other universities, where students can interact with colleagues in their fields. Upon completing their education, they find a multitude of unique employment opportunities in academia, private industries, public institutions and government agencies.



#### ■ Research with major impact

Research in the department addresses problems of foremost societal significance and vital economic importance. Major topics addressed encompass sustainable energy production, storage and transmission, the environment, homeland security, health, catalysis, semiconductors, separations, nanoparticles and process synthesis. Studies are both fundamental—generating new knowledge, and applied—developing new processes and technologies. The research advances existing industries and spawns new enterprises. Graduates from the program are capable of becoming leaders in their respective fields of choice.

### 2012 chemical engineering M.S. and Ph.D. awards

- **Trevor Ault** (M.S.), A Techno-Economic Analysis of Ethanol Production from Hydrolysis of Cellulose with Nanoscale Magnetic Solid-Acid Catalysts
- **Benjamin Clubine** (M.S.), Synthesis and Characterization of Bulk Single-Crystal Hexagonal Boron Nitride from Metal Solvents
- **Dale Green** (M.S.), A Probabilistic Approach to Reaction-Coordinate and Rate-Constant Modeling Applied to Epoxide Ring-Opening Reactions
- **Lydia R. Stefanik** (M.S.), Literature Review of Inorganic Ultraviolet Radiation Filters
- **Ronald Michalsky** (Ph.D.), Thermochemical Production of Ammonia Using Sunlight, Air, Water and Biomass
- **Xin Sun** (Ph.D.), Fundamental Research of the Solvent Role in the Ionothermal Synthesis of Microporous Materials
- **Fan Zhang** (Ph.D.), Development and Scale-Up of Enhanced Polymeric Membrane Reactor Systems for Organic Synthesis





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