Annual Report 2011 Chemical Engineering

COLLEGE OF ENGINEERING



KANSAS STATE



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MESSAGE FROM THE DEPARTMENT HEAD

Tt is a pleasure for me to present the Latest accomplishments of the faculty and students of the chemical engineering department at Kansas State University. The department continues to makes advances in its areas of expertise, including sustainable energy and chemical production, advanced materials technologies, homeland security, health and the environment. These new technologies are established in an atmosphere that provides great educational and learning experiences for our undergraduate and graduate students. Highlights for the department in 2011 are summarized here; the details can be found in this annual report.



Vikas Berry achieved numerous research milestones in 2011. He received a prestigious NSF CAREER award for

faculty early in their academic career, the only such award made in the state of Kansas in 2011. He also received two additional grants in 2011, from the Office of Naval Research and MEMC, Inc., all in support of his research on graphene, a recently discovered, atomically thin, two-dimensional layer of carbon with extraordinary physical and mechanical properties.

The department's research on energy and sustainability continues to grow. New research grants received in 2011 included a research experience for undergraduates (REU) grant on bioenergy, directed by Mary Rezac; bimetallic nanoparticle catalysts for reforming hydrocarbon fuels, directed by Keith Hohn; and funding to study the conversion of biomass to butylenes, also directed by Keith Hohn. The department now has two REU centers; the second is on sustainable energy, codirected by Larry Erickson and Keith Hohn. L.T. Fan and his former student Tengyan Zhang contributed two major chapters on sustainability to appear in the monograph Recent Advances in Sustainable Process Design and Optimization.

Since 2007, the department has admitted primarily Ph.D. candidates in an effort to improve its research reputation. As a consequence, in 2011 seven Ph.D. degrees were awarded, the largest number ever for the department in a single year. These students received numerous awards and recognitions including two Global School of Advanced Studies awards, to Nihar Mohanty and Kabeer Jasuja, which are given annually to the top graduate students in the world.

Our faculty, undergraduate students and alumni also received honors recognizing their accomplishments. Senior Andrew Saterlee, who worked with John Schlup on cancer treatments,



received a National Science Foundation Graduate Research Fellowship. Mary Rezac and alumnus Sigifredo Castro Diaz (M.S. 2001, Ph.D. 2003) were both listed in the top 150 scientists in Kansas in the past 150 years by Ad Astra Kansas.

The research reputation of the faculty and students continues to grow. Publications authored or co-authored by them were cited more than 1,200 times in 2011 in the scientific literature. Graduate students helped to disseminate research results through posters and presentations at numerous professional meetings including the AIChE, ACS, the North American Membrane Society, Gordon Research Conference, the Electrochemical Society, the K-State Research Forum and the K-State Bioenergy Symposium. Students draw

from the expertise they gain by working with many departments outside of chemical engineering-chemistry, mechanical and nuclear engineering, biological and agricultural engineering, and grain science and industry, as well as other universities and national laboratories such as the Naval Research Laboratory and Oak Ridge National Laboratory.

The department's research facilities will dramatically improve in 2012, thanks to a recent NSF grant. Half of the CHE laboratories in Durland Hall will be renovated and expanded in size to provide new capabilities and a better, safer work environment. As part of this change, all graduate student offices were moved from Durland Hall to newly furnished offices in Seaton Hall. The renovation will be completed in fall 2012.

The state of Kansas has initiated an ambitious program to expand the number of engineering graduates produced by its major universities by 30% over the next 10 years. We are excited by this University Engineering Initiative Act, and the department looks forward to taking advantage of the teaching and research opportunities it will create.

Additional information on our department can be found on our website at www.che.ksu.edu. We welcome your interest.

James N. Edgar

James H. Edgar Department Head Chemical Engineering



Vikas Berry: The new shape of technology

Engineering research uses graphene to form tomorrow's electronics

Graphene research at Kansas State University is taking many shapes: dots, cloaks, ribbons, snowflakes and more.

Vikas Berry, the William H. Honstead professor of chemical engineering, is fabricating these shapes from graphene, a form of carbon that is only one atom thick. He is using it to improve electronics, optoelectronics and computers.

Berry's recent project — supported by a five-year \$400,000 National Science Foundation CAREER award — focuses on graphene quantum dots, which are ultra-small sheets of carbon atoms. Berry's eight-member research team is controlling the size of these graphene particles and shaping them into squares, triangles, rectangles or ribbons. By doing so, they can control graphene's properties over a wide range to develop transistors for future computers, to manipulate graphene-based devices

and to engineer

novel graphenic

nano-systems.

The work will

be published in

issue of Nature

Communications.

"Several of the

an upcoming

Since their quantum mechanical ne, properties evolve from their shape and size, these quantum dots could be incorporated into several optoelectronic

sizes are unprecedented," Berry said.

"Our group is the first to synthesize

these quantum dots with a wide variety

of controlled structure in large quantities.

applications, including solar cells." Because of the high electronic mobility in graphene, it may lead to ultrafast computers, making it a hot topic in the semiconductor industry. Berry has received support from MEMC Electronic Materials, a Missouri-based global supplier of electronic materials to the semiconductor and solar industries, to develop ideas to integrate graphene with silicon. Berry and Mike Seacrist, senior fellow at MEMC, have jointly filed for a patent on this project.

Recently, Berry's team created a microscopic graphene cloak that protects

Because of the high electronic mobility in graphene, it may lead to ultrafast computers, making it a hot topic in the semiconductor industry.

graphene quantum dots of shapes — like squares and rectangles — and of defined

bacteria and other cells under an electron microscope so they can be imaged at their natural size with higher resolution. Their work with graphene cloaks appeared in the journal Nano Letters in 2011. Now the team is

using bacterial biochemical processes to create fine wrinkles on the graphene.

"This can be an important breakthrough, since the wrinkles and the associated strain open a band gap in graphene, making it advantageous to fabricate graphene transistors with high rectification," Berry said. "The next step is to compare graphene devices with and without wrinkles to evaluate the effectiveness of the process for future incorporation into devices." Berry has several other recent projects and

Berry has several other recent projects and accolades related to graphene.

He has received \$300,000 from the Office of Naval Research to study tapered ribbons of graphene, which have important electrical properties.



He is currently collaborating with Zhiping Xu from Tsinghua University in China to conduct simulations on the process to produce quantum dots. Berry is also working with Vivek Shenoy from Brown University to study molecular motion on graphene's surface.
He has a \$301,700 National Science Foundation-funded project on a route to functionalize graphene.
Berry's team has imbedded gold "snowflakes" on graphene to make it more useful in electronic applications.

—By Jennifer Tidball K-State Communications and Marketing



James H. Edgar

• Department Head and Professor

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

- Assistant 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 liguids
- Teaching: Thermodynamics, separational process design, transport phenomena laboratory



Vikas Berrv Assistant Professor

- 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 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, 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 ChE, bioseparations, separational process design, biochemical engineering

Mary E. Rezac



• Professor

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, process dynamics and control





RESEARCH

Kansas State Chemical Engineering **Research Areas**

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, defectfree 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

Principal interests in this study concern the interaction of tur-A multi-disciplinary collaboration between Drs. Amanorbulence with fluid-borne entities in multi-phase processes. Specific Boadu (agricultural economics), Nelson (resources) and Pfromm areas of study include flocculation, aggregate breakage, aggregate (engineering) has resulted in an initial publication on the deformation, expulsion of interstitial fluid from floc structures and technological sustainability of algae-based diesel that has found effects of oscillatory fluid motions upon interphase transport. In some resonance. Several publications have already taken note of addition, investigation includes bubble formation, coalescence and





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

Transport Studies in Chemical Engineering



breakage in aerated reactors, the effects of energetic interfacial phenomena upon cells in culture, and the impulsive distribution of small particles in airfilled chambers. A study has also been initiated on the effectiveness of a passive mixing device for the treatment of agricultural waste waters.

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 converting 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-percursor 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 synthesizatjion 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.

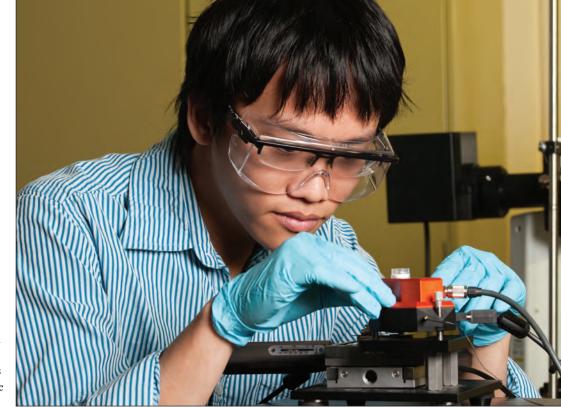
Dr. Keith Hohn



Crystal Growth and Epitaxy of Boron Compound Semiconductors

Semiconductors are the key component in many solid-state devices including Blu-ray 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 (B₁₂As₂), 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 ten thousand 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 with 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 siliconbased electronic devices, because they enable large voltage swings and result in greatly reduced 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 $(A_{12}O_3)$ 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 that are 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 metalcoordination bonds, (c) nanostructured into quantum dots and nanoribbons, (d) composited with biocompatible polymer to produce bacterial repellant 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. There are several research problems related to air emissions and liquid and solid effluents from



industrial and agricultural processes. One current problem is the 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

PUBLICATIONS

Jennifer L. Anthony

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- Sun, X. and J.L. Anthony, "Influence of Structural Variation in Imidazolium-Based Ionic Liquids on SiO2 Particle Saturation Points," J. Phys. Chem.. C, accepted.

Vikas Berry

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James H. Edgar

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- Whiteley, C.E., Y. Zhang, Y. Gong, S. Bakalova, A. Mayo, J.H. Edgar, and M. Kuball, "Semiconducting Icosahedral Boron Arsenide Crystal Growth for Neutron Detection," J. Cryst. Growth 318 553 (2011).
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Larry Erickson

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L. T. Fan

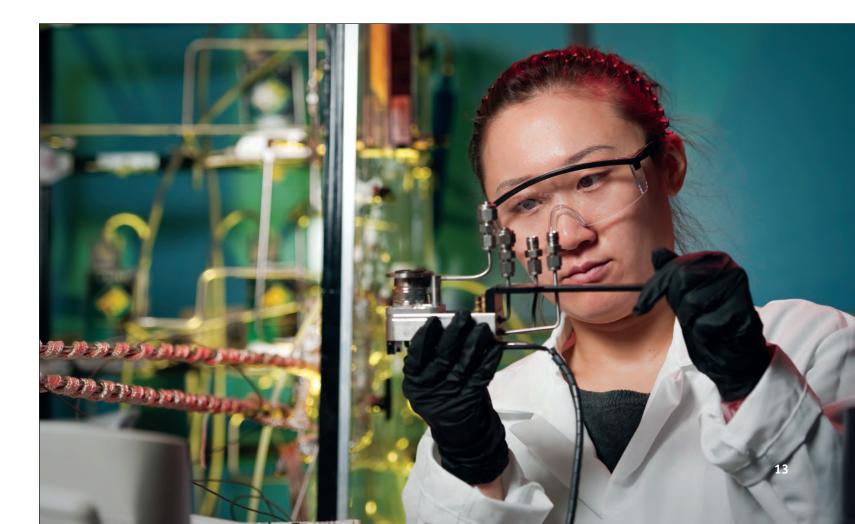
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of Transportation," Clean Tech. Environ. Policy, 13, 637-642 (2011).

Fan, L. T., A. Argoti, and S. T. Chou, "Stochastic Modeling for the Formation of Activated Carbons: Nonlinear Approach," Ind. Eng. Chem. Res., 50, 8836-8841 (2011).

Larry A. Glasgow

- Created text for introductory course in advanced engineering mathematics, CHE 735, Chemical Engineering Analysis 1. This course is specifically designed to address the needs of graduate students with regard to preparation for work required in CHE 850 and CHE 862-867. Four book chapters (including problems) have been completed.
- Algebraic Equations
- Numerical Solution of Ordinary Differen tial Equations
- Analytic Solution of Partial Differential Equations
- Numerical Solution of Partial Differential Equations



D.E., "Experimental and theoretical analysis of a novel deep-bed solid-state bioreactor for cellulytic enzymes production," Biochemical Engineering Journal, 58-59, 110-123 (2011). Boyle, D., Sun, X.S., and Wang, D., "Cellobiose hydrolysis using acid-functionalized nanoparticles," Biotechnology and Bioprocess Engineering, 16, 1214-1222 (2011).

Brijwani, K., Vadlani, P.V., Hohn, K.L., Maier, Pena, L., Ikenberry, M., Ware, B., Hohn, K.L.,

Cruz, J. C., Würges, K., Kramer, M., Pfromm, P. H., Rezac, M.E., Czermak, P., "Immobilization of Enzymes on Fumed-Silica Nanoparticles for Applications in Nonaqueous Media," in: Wang, P. (ed.), Nanoscale Biocatalysis, Methods and Protocols; Series: Methods in Molecular Biology, vol. 743, Springer/Humana Press, May 2011, ISBN 978-1-61779-131-4.

Hussain, M. A. M., Anthony, J. L., Pfromm, **P. H.**, "Reducing the energy demand of corn-

Keith L. Hohn

Peter H. Pfromm



based fuel ethanol through salt-extractive distillation enabled by electrodialysis," AIChE Journal (Impact Factor 1.96, 2011), doi: 10.1002/ aic.12577, 2011.

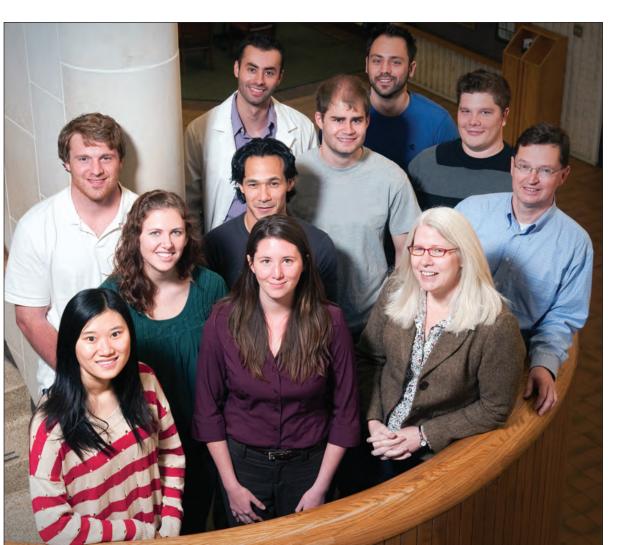
- Justice, C., Brix, A., Freimark, D., Kraume, M., Pfromm, P., Eichenmueller, B., Czermak, P., "Process Control in Cell Culture Technology Using Dielectric Spectroscopy," Biotechnology Advances (Impact Factor 8.25, 2011), 29(4), 391-401, 2011.
- Michalsky, R., **Pfromm, P. H.**, "Chromium as reactant for solar thermochemical synthesis of ammonia from steam, nitrogen, and biomass at atmospheric pressure," Solar Energy (Impact Factor 2.01, 2011), 85, 2642-2654, 2011.
- Parman, B. J., Amanor-Boadu, V., Pfromm, P. H., Michalsky, R., "Third-Generation Biofuels and the Food versus Fuel Debate: A Systems Perspective," The International Journal of Environmental, Cultural, Economic and Social Sustainability (new journal, no impact factor assigned), 7(2), 287-300, 2011.
- Pfromm, P. H., Amanor-Boadu, V., Nelson, R. G., "Sustainability of algae-derived biodiesel: a

mass balance approach," Bioresource Technology (Impact Factor 4.25, 2011), 102(2), 1185-1193, 2011.

■ Singh, D., Rezac, M.E., Pfromm, P. H., "Overcoming mass-transfer limitations in partial hydrogenation of soybean oil using metal-decorated polymeric membranes," AIChE Journal (Impact Factor 1.96, 2011), 57(9), 2450-2457, 2011.

Mary E. Rezac

- Cruz, J. C., Würges, K., Kramer, M., Pfromm, P. H., Rezac, M. E., Czermak, P., "Immobilization of Enzymes on Fumed-Silica Nanoparticles for Applications in Nonaqueous Media," in: Wang, P. (ed.), Nanoscale Biocatalysis, Methods and Protocols; Series: Methods in Molecular Biology, vol. 743, Springer/Humana Press, May 2011, ISBN 978-1-61779-131-4.
- Singh, D., Rezac, M., Pfromm, P.H., "Overcoming Mass-Transfer Limitations in Partial Hydrogenation of Soybean Oil Using Metal-Decorated Polymeric Membranes," AIChE Journal, vol. 57(9), pg. 2450-2457, 2011.



GRANTS



Jennifer Anthony

- Co-PI (with Timothy I. Morrow, LA Tech), "Synthesis of Nanoporous Zeolitic Materials in Ionic Liquids: A Fundamental Study of the Solvent's Role," Submitted to the National Science Foundation, \$274,966 over three years (JLA share: \$249,724) Funding Period: August 2008 – July 2011.
- 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.

Vikas Berry

- PI, "Tapered Graphene Nanoribbons of Controlled Width and Tapering Angle: Carrier-Tunable Diodic Transistor." Office of Naval Research; Amount \$300,000; Start Date: 07/01/11; 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.
- PI, "Detection of Cancer Market with Graphene Sensors." Terry C. Johnson Center for Basic Cancer Research; Amount \$25,500; Start Date: 04/01/10; Period = 1 Year.
- 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

- "High-K Oxide Insulating Gate Group III Nitride-Based FETs," Department of Defense Experimental Program to Stimulate Competitive Research (DEP-SCoR), 2010-2013, \$452,710.
- ARI-MA: Collaborative Research: "Hexagonal Boron Nitride-Based Neutron Detectors," National Science Foundation, 2010-2015, \$961, 788 (KSU portion), with J. Geuther (KSU) and Texas Tech University.



- "Materials Development of Boron Phosphide-Based Neutron Detectors," Department of Energy, 2010-2012, \$560,000.
- 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).
- "Bulk Crystal Growth and Epitaxy of Icosahedral Boron Arsenide," II-VI Incorporated Foundation, 2008-2011, \$207,900.
- "Durable betavoltaic devices based on boride semiconductors," Expeditionary Capabilities Consortium, M2 Technologies, 2010-2011, \$61,850.50.
- "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

- "Westar Wetlands Pilot Project," Westar and Burns and McDonnell, with Stacy Hutchinson, Ganga Hettiarachchi, and Larry Davis. \$377,524, 2 years.
- U.S. Department of Defense Subcontract with M2 Technologies for the Urban Operations Laboratory, 2002 to the present, with James Guikema, Blase Leven, Steve Eckels, Keith Hohn, Jennifer Anthony, Larry Glasgow, and others.
- Co-PI (with Keith Hohn), NSF REU "Earth, Wind, and Fire: Sustainable Energy for the 21st Century."
- NSF EPSCoR "Climate Change and Energy: Basic Science Impacts and Mitigation," K. Bowman James is PI with investigators at KU, KSU, and WSU.
- (with Ganga Hettiarachchi, Sabine Martin, Blase Leven, and others), EPA "Sustainable Gardening Initiatives at Brownfield Sites."
- Co-PI (with Larry Davis), "Mango Remediation," Remediation of Chlorinated Solvents in Soil and Groundwater.
- (with James Guikema, Blasé Leven, Steve Eckels, and others), New funding from M2 Technologies and U.S. Department of Defense for the Expeditionary Capabilities Consortium.

L. T. Fan

 "Mitigating Pollutant and Pathogen Contamination in Livestock Operations," Ronaldo G. Maghirang (50%) and L. T Fan (10%), AES, 10/1/2010-9/30/2015.

Larry A. Glasgow

 "Remote Vehicle Stopping—Rapid Engine Suffocant," M2 Technologies-USMC, \$75,000 for FY 2009. The project end date is January 2011.

Keith L. Hohn

- 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, \$100,000 (my share is about two-thirds: GRA will be supported out of chemical engineering), 1/11-12/13.
- Co-PI (with Larry Erickson), NSF, "REU Site: Earth, Wind, and Fire: Sustainable Energy for the 21st Century," \$269,445, 3/09-2/12.
- 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, potential support for one GRA (stipend and tuition) for 4-6 years out of \$3,171,485, 09/09-06/14.
- Senior personnel (with PIs Jun Li, Judy Wu, and Francis D'Souza), "Nanotechnology for Renewable Energy," NSF EPSCoR, \$14,000 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.

Peter H. Pfromm

- PI, "Topics in Antigen Production," Böhringer Ingelheim Vetmedica Inc., St. Joseph, Missouri, 2008-2011, \$141,221.
- PI (with M.E. Rezac, 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.E. Rezac), "Membrane reactor technology for the efficient conversion of biomass to industrial chemicals," USDA AFRI, \$587,000 (50% to Pfromm), 2010-2013.
- Co-PI (with M.E. Rezac, and J. Edgar), "Sustainable energy solutions via systems-based research: a proposal to modernize the sustainable energy research infrastructure in Durland Hall," NSF, 2010-2012, \$1,998,850.

Mary E. Rezac

- PI, Membrane Reactor Evaluation for Specialty Chemicals Production: Phase II, DOE SBIR Program, Joint with Compact Membrane Systems, \$750,000 (\$196,000 to KSU), November 2007–March 2011.
- PI, Membrane Reactor Evaluation of Transesterification Reactions: Phase II, DOE STTR Program, Joint with Compact Membrane Systems, \$750,000 (\$225,000 to KSU), August 2008–August 2012.
- Co-PI (with Ron Madl and Richard Nelson), Center for Sustainable Energy Education and Research, KSU Targeted Excellence, \$750,000, August 2007–July 2011.
- PI (with Maier and Maes), Biobased Products and Bioenergy Multi-University Graduate Program, USDA, \$498,290, August 2009–July 2012.
- PI (with Peter Pfromm, Jeff Peterson, Kyle Douglas-Mankin, Co-PIs), IGERT: From crops to commuting: integrating the social, technological, and agricultural aspects of renewable and sustainable biorefining (I-STAR), NSF, \$3,171,485, September 2009–August 2014.
- PI, Kansas State University Center for Sustainable Energy, ConocoPhillips via the KSU foundation, \$750,000, October 2009–September 2014.
- PI (with Pfromm co-PI), Membrane Reactor Technology for the Efficient Conversion of Biomass to Industrial Chemicals, USDA, \$587,000, December 2010–November 2013.
- PI (with Madl co-PI), Kansas State University Center for Sustainable Energy, \$1,213,625, (DoE); \$241,000 (KSU match), November 2010–October 2012.
- PI (with Pfromm and Edgar Co-PIs), Sustainable Energy Solutions via Systems-Based Research: A Proposal To Modernize the Sustain-

able Energy Research Infrastructure in Durland Hall, NSF, \$1,598,997, October 2010 – September 2013.

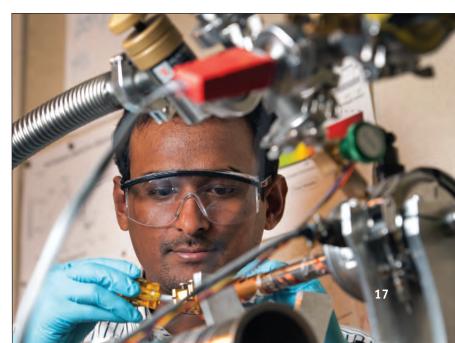
John R. Schlup

PI (with James L. Neihart), "Simulation of the Impact of Input Parameters and the Effectiveness of Boron Neutron Capture Therapy (BNCT)" (Undergraduate Cancer Research Award), Johnson Center for Basic Cancer Research (Kansas State University, 2009–2010 academic year, \$1,000. Renewed for 2010 – 2011 academic year).

PI (with Patrick C. Shriwise), "Boron Neutron Capture Therapy (BNCT) Employing Stem Cells as Boron Carriers: Determination of Boron Density Using Neutron Activation Analysis (NAA)" (Undergraduate Cancer Research Award), Johnson Center for Basic Cancer Research (Kansas State University, 2009–2010 academic year, \$1,000. Renewed for 2010 – 2011 academic year).

PI (with Andrew B. Satterlee), "Synthesis of Boron-Containing Compounds for Attachment to Stem Cells" (Undergraduate Cancer Research Award), Johnson Center for Basic Cancer Research (Kansas State University, 2009–2010 academic year, \$1,000. Renewed for 2010 – 2011 academic year).

 PI, "Online Courses on Biorenewable Resources and on Engineering Sustainability," US Department of Transportation (Sun Grant Initiative – South Central), 7/1/09 – 6/30/11, \$77,075.



18

PROFESSIONAL

service/recognition

Jennifer Anthony

- Member, American Institute of Chemical Engineers
- Member, Area 1a planning committee
- Member, American Chemical Society ■ Member, Sigma Xi Research Society
- Member, American Society of Engineering
- Education
- Member, Materials Research Society
- Member, International Zeolite Association
- Member, International Congress on Ionic Liquids (COIL-4) Planning Committee
- Reviewer, various journals

Vikas Berry

- NSF-CAREER Award
- William H. Honstead Professorship of Chemical Engineering
- Plenary lecturer, Tsinghua University in China
- Nominee, ECS Young Investigator Award and Frankenhoff Research Award
- Member, editorial board, Nature Publication Group journal: Scientific Reports
- Member, NSF panel, CMMI
- External reviewer, Wayne State University, Research Enhancement Program in Physical Sciences
- Reviewer, various scientific articles
- Chair, AIChE, "Graphene and Carbon Nanotube-Based Devices"
- Chair, AIChE, "Integration of Biological Systems with Electronic and Photonics"
- Member, editorial board, Journal of Nanoscience Letters
- Member, advisory board, All Results Journal-Nano

James H. Edgar

- Reviewer, manuscripts for five journals
- Collaborator, Naval Research Laboratory
- Member, NSF Major Research Instrumentation Panel

Larry Erickson

- Member, International Phytotechnology Society Board of Directors
- Reviewer, various proposals and manuscripts
- Treasurer, Environmental Division of AIChE

- Treasurer, Chemical Engineering and Law Forum of AIChE
- Member, Environmental Progress and Sustainable Energy Editorial Board
- Member, International Journal of Phytoremediation Editorial Board
- Session chair, AIChE Annual Meeting

L. T. Fan

- Member, scientific committee, Gulf Coast Hazardous Waste Research Center
- Participant, University Distinguished Professors' Forum
- Reviewer, various manuscripts for technical journals and miscellaneous research proposals

Larry A. Glasgow

- Reviewer and technical adviser, KLAenviro
- Provisional patent applicant and presenter, vehicle-stopping project for WBT Showcase

Keith L. Hohn

- Session co-chair (2), North American Catalysis Society 22nd Annual Meeting
- Editor-in-chief, Catalysts, international peerreviewed online journal
- Member, NSF panel: SBIR Phase I (catalytic processes)
- Reviewer, numerous journals and proposals

Peter H. Pfromm

■ Presenter, Science Cafe, Sigma Xi scientific research society lecture series

Mary E. Rezac

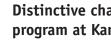
- President, North American Membrane Society
- Director, North American Membrane Society
- Member, external advisory board, Clemson University Department of Chemical Engineering
- Member, scientific advisory committee, International Congress on Membranes

John R. Schlup

- Evaluator, ABET Program Candidate Training
- Candidate, AIChE, ABET Program Evaluator
- Presenter, "A 'Seven-Trait Writing Tool' for Assessment of Technical Writing," ABET Symposium

GRADUATE STUDIES

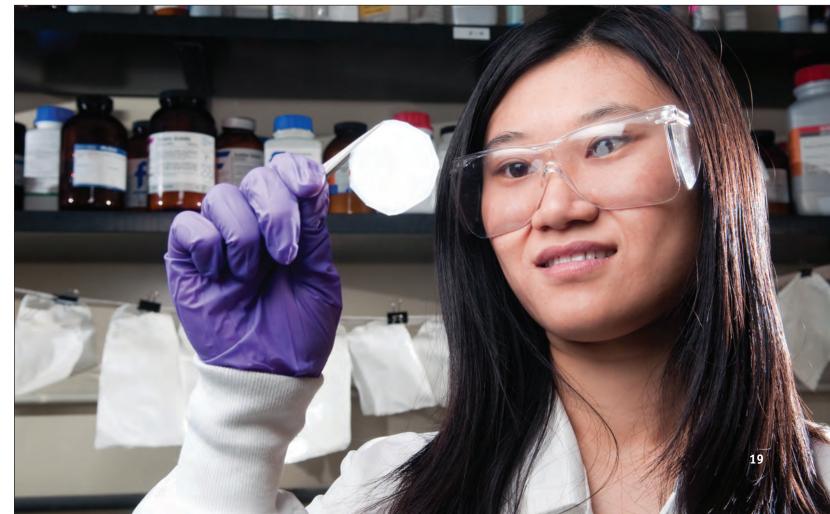




Strong financial support for graduate students

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



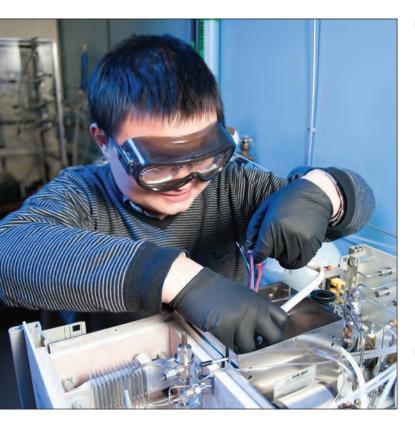
Distinctive characteristics of the chemical engineering graduate program at Kansas State University include the following:

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. In the fall of 2010, the ratio of Ph.D. to M.S. candidates was 10:1.

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. More than 75% of the papers from the department in 2010 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.

CONTACT INFORMATION



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 advisors 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.

2011 chemical engineering Ph.D. awards

Alex Brix, Vaccine Production

Li Du, Bulk Crystal Growth, Characterization and Thermodynamic Analysis of Aluminum Nitride and Related Nitrides

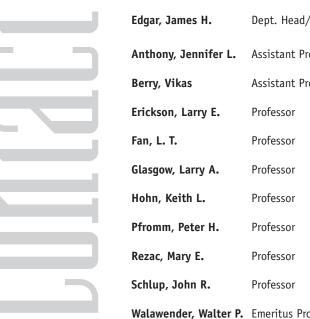
Mohammed Hussain, Salt-Extractive Distillation Using Electrodialysis

Kabeer Jasuja, Designing Nanoscale Constructs from Atomic Thin Sheets of Graphene, Boron Nitride and Gold Nanoparticles for Advanced Material Applications

Nihar Mohanty, Structural and Chemical Derivatization of Graphene for Electronics and Sensing

Clinton E. Whiteley, Advanced Crystal Growth Techniques with III-V Boron Compound Semiconductors

Yi Zhang, Epitaxial Growth of Icosahedral Boron Arsenide on Silicon Carbide Substrates: Improved Process Conditions and Electrical Properties





/ Professor	Durland 1005	785-532-5584	edgarjh@ksu.edu
rofessor	Durland 1018	785-532-4321	anthonyj@ksu.edu
rofessor	Durland 1011	785-532-5519	vberry@ksu.edu
	Durland 1012	785-532-4313	lerick@ksu.edu
	Durland 2045	785-532-4327	fan@ksu.edu
	Durland 1013	785-532-4314	glasgow@ksu.edu
	Durland 1016	785-532-4315	hohn@ksu.edu
	Durland 1036	785-532-4312	pfromm@ksu.edu
	Durland 1017	785-532-4317	rezac@ksu.edu
	Durland 1039	785-532-4319	jrsch@ksu.edu
ofessor	Durland 1019	785-532-4318	walawen@ksu.edu
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College of Engineering

Chemical Engineering

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Notice of nondiscrimination

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