# College of Engineering

# *2013 Annual Report*

## Chemical Engineering

KANSAS STATE
UNIVERSITY

# Contents



# Message from the department head

In helping the university fulfill K-State's 2025 visionary plan to become a Top 50 public research university, the department is placing great emphasis on its research. Indeed, we are a research-intensive department. Our annual research expenditures of $4.7M are the largest in the engineering college at K-State, and the highest rate per tenured or tenure-track faculty. Through our research, the chemical engineering department seeks solutions to major societal problems such as clean and sustainable energy, environmental remediation and homeland security. Of equal importance is the excellent educational opportunity that research provides our students. Students are trained on state-of-the-art equipment, learn to work independently and collaborative, study background information in depth, learn to be detail-oriented, tolerate frustration, optimize their experiments, organize their results, identify important trends, draw insights, and learn how to present their work in interesting and compelling manners, both in writing and orally, in reports and presentations. Via their research, students learn how to solve open-ended problems subject to many different variables for which multiple solutions may exist. Their involvement in planning, supervising and presenting research also ensures our faculty remains current in important chemical engineering topics.

Our core research studies are performed and driven by our graduate students, almost all of whom are Ph.D. candidates. In large part, they keep the experiments and simulations running, and set the priorities to achieve the research objectives. Almost all of our graduate students advise and are helped by undergraduates. A research experience is now required of all of our undergraduate students through the senior laboratory class, CHE 545, Unit Operations. The seniors generally work under the direction of graduate students. Even our freshmen get a taste of research, as they are asked to investigate a chemical engineering topic or process, and give a presentation on their findings. In the summer, the department has two, NSF-supported Research Experiences for Undergraduates sites, which together host more than 20 undergraduate students researching various aspects of sustainable energy and bioenergy. To add depth and breadth to our research, the department hosts many outstanding seminar speakers who introduce our students to topics of current research.

In 2013, two new faculty members joined the department, adding to our research expertise and capabilities. Placidus Amama is focusing on the synthesis, processing and characterization of nanocarbon (such as carbon nanotubes and graphene) hybrid structures, which have applications in lithium ion batteries, catalysis and thermal management. Bin Liu calculates the energetics and most stable reactive intermediates using the first principles theory, for the analysis of heterogeneous catalysts. Both are off to a good start on their research.

In this annual report you will read about our research and related activities. We hope you find this informative and that it encourages you to find more details on our website at che.ksu.edu. Please contact us if you need additional information or would like to comment on this report.

James H. Edgar
Chemical Engineering Department Head
Tom H. Barrett Faculty Chair
University Distinguished Professor

# New faculty

Two new assistant faculty join the chemical engineering department in fall 2013

### Placidus Amama

Placidus Amama came to Kansas State University because it offered him the opportunity to pursue creative research and teaching aimed toward making a difference in the future of chemical engineering. His research interests center on nanomaterials, heterogeneous catalysis, energy storage and environmental remediation.

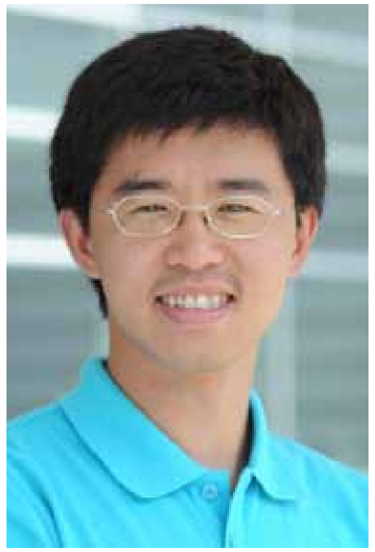
Amama's research group is focusing on rational catalyst design for the controlled synthesis of nanomaterials and hybrid nanomaterials. These nanomaterials can be used for improved energy storage in lithium ion batteries and supercapacitors, and for thermal management in electronic devices. The research has substantial scientific interest, societal need and intellectual challenge.

"I hope to help train the next generation of chemical engineers, and to impact society in a positive way through scientific discoveries and the development of new technologies," Amama said.

He received his doctoral and master's degrees in environmental engineering from Yokohama National University, and his bachelor's degree in chemistry from the University of Calabar. Amama was a research scientist with the Air Force Research Laboratory from 2007 to 2013.

Amama has more than 30 publications, and has authored more than 40 conference proceedings and presentations. He has given more than 17 invited presentations. He serves on the editorial boards for Advanced Chemical Engineering Research, Conference Papers in Materials Science and the Journal of Catalysts. Amama is a recipient of the 2014 Kansas State University Mentoring Fellowship and the 2014 Air Force Summer Faculty Fellowship Program award.

### Bin Liu



Bin Liu's research interests span the spectrum of density functional theory, molecular simulations, heterogeneous catalysis, novel catalyst materials and renewable energy.

Liu is studying complex reaction networks related to biomass-derived compounds on transition metal surfaces using density functional theory, and he also is interested in modeling the growth mechanisms of nanoscale materials for heterogeneous catalysis and next-generation electronic device applications. Liu's research group is developing new computational techniques to assist in studying complex chemical and physical processes, and correlate structural-properties relationships.

"Being at K-State gives me the perfect opportunity to fulfill my passions in teaching and carrying out multi-disciplinary research in my field," Liu said.

He received his doctoral degree in chemical engineering from Colorado School of Mines and his bachelor's degree in chemical engineering from the Dalian University of Technology. He was a research associate at Argonne National Laboratory from 2010 to 2013.

Liu has published numerous journal article and books chapters on his research, and presented at national and international conferences. He also serves as a grant reviewer and referee of several academic journals. He is a member of the American Institute of Chemical Engineers, the American Chemical Society and the American Academy for the Advancement of Science.





# Edgar named University Distinguished Professor

In 2013, James H. Edgar, department head and Tom H. Barrett professor in chemical engineering, was named a Kansas State University Distinguished Professor — the highest honor the university bestows on its faculty. It is awarded following a university-wide nomination and selection process conducted by the provost. Edgar is the second University Distinguished Professor named in the department, following L.T. Fan.

Edgar has pioneered research on the crystal growth, epitaxy, characterization and device fabrication of wide-band-gap semiconductors, including nitride (GaN and AlN) and boride (BP and BN) compounds rather than the more common silicon. These materials are used in microelectronic devices such as laser diodes, light-emitting diodes and radiation sensors, and have applications in communications, transportation, lighting, medicine and consumer products.

Edgar has received more than $9 million in research funding from the National Science Foundation, U.S. Department of Defense and U.S. Department of Energy. He has authored or co-authored more than 150 papers in scientific journals, edited two books, and presented more than 25 national and international lectures. His awards include the William H. Honstead Professor in Chemical Engineering, the Commerce Bank Distinguished Graduate Faculty Award, College of Engineering Research Excellence Award, Making a Difference Award, and the Sigma Xi Outstanding Scientist Award. He spent sabbaticals at the Naval Research Laboratory (1995) and Radbound University in the Netherlands (2006).

At the university, Edgar has advised 27 advanced-degree students and directed the research of 22 undergraduate students. He is a member of the program assessment coordination committee, graduate college assessment review committee and chair of the chemical engineering graduate students committee. He also has served on the graduate council. He has taught nine different undergraduate courses and five different graduate courses. He has been a symposium organizer for the Materials Research Society, a National Science Foundation review panelist and a reviewer for NASA's postdoctoral program, among others.

Edgar joined the university in 1988 as an assistant professor. He earned his bachelor's degree from the University of Kansas in 1981 and his doctorate from the University of Florida in 1987, both degrees in chemical engineering. He is a native of Hutchinson, Kansas.

### James H. Edgar

Department Head and University Distinguished Professor
Tom H. Barrett Faculty Chair

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

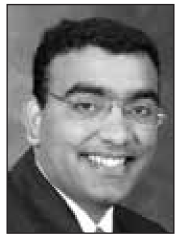
Research: Application of chemical engineering to semiconductor processing
Teaching: Engineering materials, thermodynamics, nanotechnology, solid-state devices, unit operations

### 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

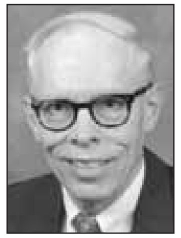


### Vikas Berry

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

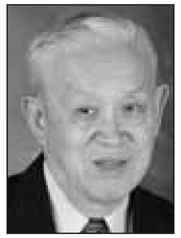


### Larry Erickson

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

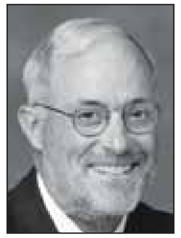


### L. T. Fan

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

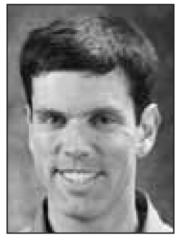


### Larry A. Glasgow

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 Sustainabilty 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. Keys to success in this field are efficient reactions and biorefining the separation of biologically derived, high-value chemicals. Compared to processing of petrochemical products, bio-based refining technology is still at its infancy. Recent efforts have focused on developing a bio-based, specific processing technology. However, the majority of 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, and presence of skin-layer defects and catalyst loading on the performance of the membrane reactor system.

Peter Pfromm
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, 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.

Peter Pfromm
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.

Peter Pfromm

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

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

Peter Pfromm
Vincent Amanor-Boadu (Agricultural Economics)
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.

Jennifer Anthony

### 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.

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).

John Schlup

### Heterogeneous Catalysis for Conversion of Biomass to Fuels and Chemicals

Heterogeneous catalysis is important for increasing the efficiency and reducing the cost to produce valuable chemicals. This is especially true for current efforts to produce industrial chemicals and fuels from renewable biomass resources. 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 a functional group and they are reusable.

Two other projects focus on use of 2,3-butanediol, a chemical that can be produced at high yield via fermentation of biomass-derived feedstocks, to chemicals and fuels. In the first project, we are reacting 2,3-butanediol and hydrogen over acid-metal bifunctional catalsyts to produce butene, which could further be converted to liquid hydrocarbons. We are the first group to study the production of butene from 2,3-butanediol, so we are exploring the catalytic properties and reaction conditions that favor butene production. We have achieved considerable success, demonstrating butene yields of 70% using a copper/ZSM-5 catalyst.

In a related project, we are exploring direct conversion of 2,3-butanediol to butadiene, an important polymer precursor. We are studying catalysts with various acid-base properties in an attempt to find a catalyst that will produce butadiene instead of methy ethyl ketone, which is the favored product at most conditions.

All projects include synthesis of 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.

Keith Hohn

### Crystal Growth and Epitaxy of Boron Compound Semiconductors

Semiconductors are key components 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 phosphide ($B_{12}P_2$), 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 phosphide. 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.

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.

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 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.

Vikas Berry

### Solar-Powered Charge Stations

Research on solar-powered charge stations for plug-in vehicles is being carried out with funding from Black and Veatch, NSF and the Electrical Power Affiliate Program. The purpose of the research is to advance science, technology, policy and sustainable development infrastructure to have parking lots filled with solar panels that generate electricity, and provide shade and shelter in support of cleaner energy production with reduced greenhouse gas emissions. A second purpose is to provide an infrastructure to charge plug-in vehicles while they are parked at work sites, shopping centers and other locations where people park. This is a multidisciplinary research effort with investigators from several other research programs.

Larry E. Erickson

### Research on Improving Soil Quality

There is a great need to improve the productivity of soil for food, biomass and related production. Miscanthus is a grass that produces large quantities of biomass and has the potential to be productive on land that needs to be improved. NATO funding has been received and a site at Fort Riley has been identified for research to investigate miscanthus production and soil quality improvement where lead and other substances from firing range training are present in the soil. K-State is working cooperatively with investigators from Ukraine and Slovakia on this project. K-State faculty in agronomy and biochemistry are working on the project, also.

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 requirements, 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

### Theoretical Understanding of Alkaline Promoter Effects in Water-Gas Shift Reaction from *Ab Initio* Methods

Hydrocarbon reforming is currently the most significant source in industrial hydrogen productions. In recent years, renewed interests arise driven by the needs, such as fuel cell technology, to develop novel hydrogen production processes. Water-gas shift reaction (also known as WGSR) is playing the central role in determining the overall process efficiency. In our group, theoretical instruments will be developed to advance our understanding aimed at improving hydrogen production efficiency from the perspective of designing novel, effective WGSR catalysts for ultimate industry-scale applications. We are trying to answer two specific questions from this study involving the role of promoter species (e.g. K, Na) common in WGSR catalysts: (i) how promoter species enhance the selectivity for the main WGSR; and (ii) will promoter species suppress the activity and selectivity of side reactions, such as methanation. Our approach is to apply density functional theory (DFT) calculations to obtain a mechanistic understanding of the WGSR on different Ni single-crystal facets, such as (111) and (211), to study the elementary reactions present in both main WGSR and side reactions that decrease hydrogen selectivity. We expect to obtain reliable thermodynamic (e.g. enthalpy, entropy) and kinetic information (e.g. activation energy) from DFT calculations, and build connections that directly link to the reaction activity and selectivity. Besides explicit DFT calculations, we are strongly engaged in developing kinetic models from molecular dynamic simulations, kinetic Monte Carlo and microkinetic models, as instruments for predictions and validations of reforming processes by accounting for various key environment parameters such as temperature, pressure, coverage, catalyst size and geometry, catalyst design and optimization.

Bin Liu

### Determination of the Molecular Structures of Novel Methane-to-Methanol Conversion Catalysts from First-Principles Method

It is highly desirable to develop a process that can transform abundant, economical materials to valuable products. Methane-to-methanol (MTM) conversion has the potential to represent such a process. However, conventional MTM processes invariably involve a first reforming step, which converts methane to carbon monoxide and hydrogen (syngas) before the methanol production. The reforming step is endothermic, energy intensive for large-scale methanol production. The objective of this project is to investigate the direct methane oxidation for controlled production of methanol in the presence of the Cu/Fe-modified ZSM-5 catalyst, which exhibits promising catalytic functionalities in a direct methane-to-methanol process with high selectivities (>85% for methanol) at mild temperatures (<200°C). The molecular structures of the active center and its surrounding environment determine the unique properties of the catalyst. However, the complex nature of such real-world catalysts presents an obstacle for general catalyst design and optimization. With first-principles modeling, our overall goal is to reveal the fundamental relationship between catalyst morphology, compositions, support acidities, geometrical cage confinement associated with the active center, and the corresponding catalytic activity and selectivity for methane oxidation. Using a combination of cluster and periodic models, each of the above topics will be addressed. As a result, this project will generate a comprehensive perspective to a potentially promising solution of a significant class of catalytic conversions.

Bin Liu

### Growth of Carbon Nanotube Carpets on Conductive Substrates for Energy Applications

The application of carbon nanotubes (CNTs) in energy storage and thermal management requires the growth of CNT arrays on highly conductive substrates, such as Cu and graphene, in order to minimize the contact resistance. So far, the growth of high-quality, well-aligned CNT carpets via chemical vapor deposition occur mainly on catalysts supported on insulators ($SiO_2$ or $Al_2O_3$); achieving similar growth on metallic substrates has remained a challenge due, in part, to their inability to stabilize the catalyst and prevent deactivation.

To improve CNT carpet growth on metallic substrates, we are focusing on developing a fundamental understanding of the interfacial properties of substrates and the various mechanistic phenomena (nucleation, growth, and termination) occurring during growth. The interfacial properties of the substrates are studied using contact angle measurement, while a combination of electron microscopic and spectroscopic techniques are used to study the evolution of the catalysts on substrates. This study is expected to benefit current efforts in rational catalyst design for controlled and efficient growth of high-quality CNT arrays on non-conventional substrates.

Placidus Amama

### 3D Nanostructured Electrodes for High-Power Lithium-Ion Batteries

Next generation lithium-ion batteries (LIBs) require significant improvements in power characteristics, stability and safety to meet energy needs of portable electronic devices. Traditional LIBs are based on a 2D planar design which clearly limits the deliverable power per unit area, mass and volume. Therefore, architectures and materials for faster ion and electron transport, and improved safety are required. Carbon nanotubes (CNTs) are one-dimensional nanostructures composed of rolled-up sheets of $sp^2$ bonded graphite with outstanding electrical, thermal and mechanical properties. A 3D CNT-based nanofoam is expected to provide a lightweight, conductive and stable structure for the deposition of high-capacity active materials. CNTs could therefore offer a new technology platform for building safer, higher power and energy LIBs.

We are focusing on fabricating an innovative 3D nanostructured electrode using CNTs as nanoscale building blocks to enable optimal performance of LIBs and lay a foundation for the adoption of 3D nanocarbon materials in a 3D LIB design. The new electrode is expected to serve as an excellent model system for studying the complex interplay in the multicomponent 3D electrode system.

Placidus Amama

# Publications

### Jennifer Anthony

- Sun, X., Barich, D.H., and Anthony, J.L. (2013). Effects of structure of ionic liquids and phosphoric acid on structure of aluminum isopropoxide. Journal of Physical Chemistry C, 117 (48), 25615-25621.
- "Infrared Spectroscopic Characterization of CIT-6 and a Family of *BEA Zeolites," S. R. Tomlinson, T. McGown, J. R. Schlup, and J. L. Anthony, International Journal of Spectroscopy 2013 (2013) Article ID 961404, 7 pages. doi: 10.1155/2013/961404.

### Vikas Berry

- T. S. Sreeprasad, Phong Nguyen, Namhoon Kim, and Vikas Berry, "Controlled, Defect-Guided, Metal-Nanoparticle-Incorporation onto $MoS_2$ via Chemical and Microwave Routes: Electrical, Thermal, and Structural Properties," Nano Letters, 13 (9), 4434-4441, 2013.
- T. S. Sreeprasad, Alfredo A. Rodriguez, Jonathan Colston, Augustus Graham, Evgeniy Shishkin, Vasanta Pallem, and Vikas Berry, "Electron Tunneling Modulation in Percolating Network of Graphene Quantum Dots: Fabrication, Phenomenological Understanding, and Humidity/Pressure Sensing Applications," Nano Letter, 13 (4), 1757–1763, 2013.
- Vikas Berry, "Impermeability of Graphene and Its Applications," Carbon, 62, 1-10, 2013.
- Phong Nguyen, Junwen Li, T.S.Sreeprasad, Kabeer Jasuja, Nihar Mohanty, Myles Ikenberry, Keith Hohn, Vivek B. Shenoy and Vikas Berry, "Covalent Functionalization of Dipole-Modulating Molecules on Trilayer Graphene: An Avenue for Graphene-Interfaced Molecular Machines," Small 9 3823-3828, 2013.
- T. S. Sreeprasad and Vikas Berry, "How Do the Electrical Properties of Graphene Change with Its Functionalization?" Small, 9, 341-350, 2013.
- Vikas Berry, "Bioelectronics on Graphene," Book Chapter for "Biosensors Based on Nanomaterials and Nanodevices," CRC Press - Taylor and Fransis Publication, 2013.

### James H. Edgar

- C.D. Frye, J.H. Edgar, I. Ohkubo, and T. Mori, J., "Seebeck coefficient and electrical resistivity of single-crystal $B_{12}As_2$ at high temperatures." Phys. Soc. Jpn. 82 095001 (2013).
- D. Wei, T. Hossain, N.Y. Garces, N. Nepal, H.M. Meyer III, M.J. Kirkham, C.R. Eddy Jr., and J.H. Edgar, J. "Influence of atomic-layer deposition temperature on $TiO_2$/n-Si MOS capacitor," ECS J Solid St. Sci. Technol. 2 N110-N114 (2013).
- C.E. Whiteley, M.J. Kirkham, and J.H. Edgar, J. , "The coefficient of thermal expansion of boron arsenide ($B_{12}As_2$) between 25 °C and 900 °C," Phys. Chem. Solids 74 673-676 (2013).
- X.K. Cao, B. Clubine, J.H. Edgar, J.Y. Lin, and H.X. Jiang, "Two-dimensional excitons in three-dimensional hexagonal boron nitride," Appl. Phys. Lett. 103 191106 (2013).

### Larry E. Erickson

- Aguilar, O.A., R. Maghirang, S.L. Trabue, C.W. Rice, and L.E. Erickson, "Laboratory Evaluation of Surface Amendments for Controlling Greenhouse Gas Emissions from Beef Cattle Feedlots," International Journal of Energy and Environmental Engineering, 4:41, pp 1-14 (2013).
- McNeary, W.W. and L.E. Erickson, "Sustainable Management of Algae in Eutrophic Ecosystems," Journal of Environmental Protection, Vol. 4, No. 11A, pp. 9-19 (2013).
- Goldin, E., L. Erickson, B. Natarajan, G. Brase, and A. Pahwa, "Solar-Powered Charge Stations for Electric Vehicles," Environmental Progress and Sustainable Energy, DOI 10. 1002/ep 11898, Published Online (2013).
- Santharam, S., L.C. Davis, and L.E. Erickson, "Biodegradation of Carbon Tetrachloride in Simulated Groundwater Flow Channels," Environmental Progress and Sustainable Energy, DOI 10. 1002/ep 11808, Published Online (2013); 33: 444-453 (2014).

### L.T. Fan

- Barany, M., B. Bertok, L. T. Fan, and F. Friedler, "Relationship between Extreme Pathways and Structurally Minimal Pathways," Bioprocess Biosyst. Eng., 36, 1199-1203 (2013).
- Bertok, B., L.T. Fan, Review of Methods for Catalytic Reaction-Pathway Identification at Steady State, Current Opinion in Chemical Engineering, **2**, 487-494 (2013).
- Garcia-Ojeda, B. Bertok, F. Friedler, and L.T. Fan, Building Evacuation Planning via Time-Expanded Process-Network Synthesis, Fire Safety J., 61, 338-347 (2013).

### Keith L. Hohn

- Salazar, J.M. and Hohn, K.L., "Partial oxidation of n-butane over a sol-gel prepared vanadium phosphorous oxide," Catalysts 3 (2013), 11-26.
- Multer, A., McGraw, N., Hohn, K., and Vadlani, P., "Production of methyl ethyl ketone from biomass using a hybrid biochemical/catalytic approach," Ind. Eng. Chem. Res. 52 (2013), 56-60.
- Walker, K., Vadlani, P., Madl, R., Ugorowski, P., and Hohn, K.L., "Ethanol fermentation from food processing waste," Environmental Progress and Sustainable Energy 32 (2013), 1280-1282.

### Bin Liu

- Bin Liu, Lei Cheng, Larry Curtiss, Jeffrey Greeley, "Effects of van der Waals density functional theory corrections on trends in furfural adsorption and hydrogenation on close-packed transition metal surfaces," Surface Science, 622, 51-59 (2014).

### Peter H. Pfromm

Hussain, M., Pfromm, P. H., "Reducing the Energy Demand of Cellulosic Ethanol through Salt-Extractive Distillation Enabled by Electrodialysis," Separation Science and Technology (Impact Factor 1.02, 2010), 48(10), 1518-1528, 2013.

### Mary E. Rezac

Schulte, L., Ballard, T., Samarakoon, T., Yao, L., Vadlani, P., Staggenborg, S., Rezac, M.E., "Increased growing temperature reduces content of multiply unsaturated lipids in oilseed crops," Industrial Crops and Products, vol. 51 (2013) 212-219.

### John R. Schlup

"Infrared Spectroscopic Characterization of CIT-6 and a Family of *BEA Zeolites," S. R. Tomlinson, T. McGown, J. R. Schlup, and J. L. Anthony, International Journal of Spectroscopy 2013 (2013) Article ID 961404, 7 pages. doi: 10.1155/2013/961404.

**Placidus B. Amama**

- "Development of 3D Nanostructured Electrodes for High-Power Lithium-Ion Batteries," University Small Research Grant (Kansas State University), 2013 -2014 academic year, $2,000.

**V. Berry**

- Tapered Graphene Nanoribbons of Controlled Width and Tapering Angle: Carrier-Tunable Diodic Transistor, Office of Naval Research; $300,000; 2011-2014
- CAREER: Detailed Characterization of Graphene Quantum Dots of Controlled Size, Shape and Chemistry, National Science Foundation, $400,000; 2011-2016

**J.H. Edgar**

- I-Corps: Hexagonal Boron Nitride for Electronic Devices, National Science Foundation, $50,000, 2013-2014
- 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, 2010-2013, $560,000
- High K Oxide Insulating Gate Group III Nitride-Based FETs, Department of Defense Experimental Program to Stimulate Competitive Research (DEPSCoR), 2010-2013, $452,710

**Larry E. Erickson**

- NSF REU, "Earth, Wind, and Fire: Sustainable Energy for the 21st Century" (with Keith Hohn and others)
- NSF EPSCoR "Climate Change and Energy: Basic Science Impacts and Mitigation" (PI K. Bowman James, with investigators at KU, KSU, and WSU)
- EPA "Sustainable Gardening Initiatives at Brownfield Sites" (with Ganga Hettiarachchi, Sabine Martin, Blase Leven, and others)
- Black and Veatch, "Building a World of Difference with Solar-Powered Charge Stations for Electric Vehicles" (with Anil Pahwa and others)
- NATO, "New Phytotechnology for CleaningContaminated Military Sites," Planning Grant, $6717 (with Valentina Pidlisnyuk, Larry Davis and others)


**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

**Keith L. Hohn**

- "REU Site: Earth, Wind, and Fire: Sustainable Energy for the 21st Century" (co-PI Larry Erickson; with Donghai Wang, Anil Pahwa, Ken Klabunde, Jennifer Anthony, Ben Champion, Jun Li, and Wendy Griswold), NSF, $316,398, 3/12-2/15
- "Nanotechnology for Renewable Energy" (PIs Jun Li, Judy Wu, and Francis D'Souza; with Cindy Berrie, Stefan Bossmann, Viktor Chikan, Chris Fischer, Javier Guzman, Siyuan Han, Dan Higgins, Ron Hui, Ryszard Jankowiak, Ken Klabunde, Teresa MacDonald, Michael Murray, Michael Overcash, Z.J. Pei, Mark Richter, D. Paul Rillema, Steve Sanders, Mark Schneegurt, Val Smith, Belinda Sturm, Susan Sun, Harold Trick, Janet Twomey, Donhai Wang, Susan Williams, Graham Wilson, and Hui Zhao), NSF EPSCoR, $28,000 out of $800,000 per year, 6/2009-5/2014
- "Acquisition of a Field-Emission Scanning Electron Microscope for Kansas State University" (PIs Vikas Berry, James Edgar, Christopher Sorensen, and Jun Li; with Dan Boyle, Stephan Bossman, Viktor Chikan, Deryl Troyer, Bruce Law, Amit Chakrabarti, Christer Aakeroy, Kenneth Klabunde, Takashi Ito, Daniel Higgins, and Krista Walton), $518,928, 1/10-1/13
- "Single-Molecule Spectroscopy for Characterization of Mesoporous Acid Catalysts" (co-PI with Dan Higgins), ACS-PRF New Directions, $100,000 (Hohn's share is about two-thirds: GRA is supported out of chemical engineering), 1/11-12/13
- "Acid-Functionalized Nanoparticles for Hydrolysis of Lignocellulosic Biomass" (co-PI with Donghai Wang), National Science Foundation, $322,999 (Hohn's share is about half), 9/10-8/13
- "From Crops to Commuting: Integrating the Social, Technological, and Agricultural Aspects of Renewable and Sustainable Biorefining(I-STAR)" (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, and Scott Staggenborg), NSF IGERT, potential support for one GRA (stipend and tuition) for 4-6 years out of $3,199,996, 09/09-06/14
- "Bimetallic Nanoparticle Catalysts for Reforming of Hydrocarbon Fuels" (with Franklin Kroh, Nanoscale Corporation), DOD STTR Phase II, $300,000, 9/11-8/13

**Peter H. Pfromm**

- PI Rezac, M. E., Co-PI's Pfromm, Mankin, and Peterson, "IGERT: from crops to commuting," National Science Foundation DGE, 2009-2014, total overall $3,171,485 from NSF
- Rezac, M. E., Pfromm, P. H. (co-PI), "Membrane reactor technology for the efficient conversion of biomass to industrial chemicals," USDA AFRI, $587,000 (50% to Pfromm), 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
- 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), 2012 – 2013 academic year, $1,000
- "Synthesis of Boron-Containing Compounds for Applications in Directed Cytotherapy for Boron-Neutron-Capture Therapy," John R. Schlup and Christopher Mehrer, Johnson Center for Basic Cancer Research (Kansas State University), 2013 – 2014 academic year, $1,000

# Graduate studies

**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 involve co-authors from other disciplines and institutions. Collaborators include 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 advanced 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.

## 2013 chemical engineering M.S. and Ph.D. awards

- **Sean Tomlinson** Ph.D., The Solubility and Secondary Structure of Zein in Imidazolium-Based Ionic Liquids, Major Professor: Jennifer Anthony
- **Liz Boyer**, M.S., A Study of Membrane Properties on Air-Conditioning Performance, Major Professor: Mary Rezac
- **MD Tashfin Zayed Hossain**, Ph.D., Electrical Characteristics of Gallium Nitride and Silicon-Based Metal-Oxide Seminiconductor (MOS) Capacitors, Major Professor: James Edgar
- **Xiaojiao Sun**, Ph.D., Single-Molecule Studies of Acidity in Heterogeneous Catalysts, Major Professor: Keith Hohn
- **David Schmidt**, M.S., Simulating Aerosol Formation and Effects in Nox Absorption in Oxy-Fired Boiler Gas Processing Units Using Aspen Plus, Major Professor: Larry Erickson

# Seminar speakers

- Kevin McCarty, Sandia National Lab, Livermore, CA, Directly Observing How Surfaces Equilibrate Bulk Defects in Materials
- Chris Depcik, Mechanical Engg, University of Kansas, Converting Detailed Kinetics into an Adaptive Global Mechanism for Automotive Catalyst Modeling
- Harvey W. Blanch, Merck Professor of Biochemical Engineering, Dept. of Chemical and Biomolecular Engineering and Joint BioEnergy Institute, University of California, Berkeley, Renewable Fuels: A Challenge for Technology or Policy?
- Christine Aikens, Associate Professor, Dept. of Chemistry, Kansas State University, Unraveling Nanoparticle Properties Using Theoretical Methods
- Jerald L. Schnoor, Professor and Allen S. Henry Chair in Engineering, Dept. of Civil and Environmental Engineering, University of Iowa, Water Sustainability in a Changing World
- Hendrik Verweij, Professor, Dept. of Materials Science and Engineering, Ohio State University, Inorganic Membranes
- David Cox, Professor and Head, Dept. of Chemical Engineering, Virginia Tech University, Reactions of Simple Alkyl and Carbene Intermediates on Transition Metal Oxide Surfaces
- Joan F. Brennecke, Keating-Crawford Professor of Chemical and Biomolecular Engineering, University of Notre Dame

**External Advisory Board**
Front row, from left: Terri Hopkins, Brad Beecher, Rick Kinder, Natalie Gosch, Brandy Reed and Ashish Ghosh; middle row, from left: J.H. Edgar, Matt Pretz, Lisa Ostenberg, Steve Hieger, Kathy Rassmussen and Laura Winks; not pictured: Jarad Daniels, Travis Rogers and Jon Wright.

**2013 Faculty**
Front row, from left: James Edgar, Jennifer Anthony, Larry Erickson, L. T. Fan and Keith Hohn; middle row, from left: Vikas Berry, Peter Pfromm, Placidus Amama, Larry Glasgow and Bin Liu; back row, from left: Mary Rezac, John Schlup and Chris Aikens.



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