Chemical and Biomolecular Engineering

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Research in the Department of Chemical and Biomolecular Engineering encompasses a wide range of fundamental specialties that advance technologies in the chemical, energy, pharmaceutical, semiconductor, biotechnology, and human health industries. The strong, science-based approaches taken by the department’s faculty provide these industries with a solid foundation on which to advance their technologies.

Our faculty members push the boundaries of engineering science. In addition to productive research programs in traditional areas in fluid mechanics, reactor engineering, catalysis, corrosion, control, and optimization, the Chemical and Biomolecular Engineering faculty have established innovative efforts in nanotechnology, biotechnology, cell and tissue engineering, drug delivery, systems biology, microchemical systems, and complex fluids. These activities sustain a leadership position in advancing technologies that affect our standard of living and improve our quality of life.

The department has an outstanding tradition of fundamental research that is well supported by a strong base of corporate, federal, and private funding. Single investigator grants remain an important component of research support, but our faculty members also play central roles in a wide range of multidisciplinary research programs across the campus. These activities are centered at the Beckman Institute for Advanced Science and Technology, the Frederick Seitz Materials Research Laboratory, the Institute for Genomic Biology, the National Center for Supercomputing Applications (NCSA), and the National Science Foundation Nanoscale Science and Engineering Center. Faculty participation in these activities is a testament to the centrality of chemical engineering fundamentals in a broad range of critical technologies. Participation in these multidisciplinary efforts also enable faculty members to leverage funding provided by the Defense Advanced Research Projects Agency (DARPA), Department of Defense (DOD), Department of Energy (DOE), the National Science Foundation (NSF), and the National Institutes of Health (NIH).

Research in Chemical and Biomolecular Engineering results from close, productive collaborations among faculty members, postdoctoral fellows, graduate students, and undergraduate students. Admission to graduate study is an extremely selective process. As part of their doctoral training, students carry out cutting-edge research in university laboratories and some participate in internships at corporate research laboratories. Joint research programs with the National University of Singapore and several research institutes in Singapore give an international accent to departmental efforts. The interdisciplinary and collaborative environment of the department provides an intellectually rich and exciting environment in which to learn and work.

The Department of Chemical and Biomolecular Engineering is in the School of Chemical Sciences in the College of Liberal Arts and Sciences.

Faculty and Their Interests

Richard C. Alkire
Electrochemical engineering

Richard D. Braatz
Multiscale systems and control

Thomas J. Hanratty, Emeritus
Fluid dynamics

Jonathan J. L. Higdon
Fluid mechanics, computational algorithms

Paul J. A. Kenis
Microfuel cells, microreactors, engineered platforms for biology, microfluidic crystallization platforms

Hyun Joon Kong
Biomaterials, cell adhesion, tissue engineering, cell

Mary L. Kraft
Phospholipid bilayers, phase-separation, secondary ion mass spectrometry, cell membrane microdomains, glycosylation
Controlled-release drug delivery systems can provide therapeutic benefits while reducing side effects and reducing the frequency of administrations. However, the design of controlled-release systems can be challenging due to incomplete understanding of the mechanisms that regulate release. We are modeling the effects of polymer particle size distribution, molecular weight distribution, pore size distribution, and the accumulation of acidic degradation byproducts on macromolecule release in biodegradable polymer drug delivery systems. A model-based optimization algorithm will be developed to design drug delivery systems to produce desired release profiles.

Microfluidic Chips for Kinetic Studies of Biochemical Processes Using FTIR Imaging
University of Illinois at Urbana-Champaign Critical Research Initiative

FTIR probes the energetics and geometries of chemical bonds and is a particularly valuable spectroscopic tool to study the conformation and structure of biological macromolecules. Time-resolved FTIR spectroscopy can provide the essential details of bond making and breaking during key biochemical processes. Such studies have been very limited due to technical difficulties arising from the very low amplitude of the measured signals. We are developing microfluidic chips that, combined with FTIR imaging microscopy, will be able to overcome these limitations. We have already been able to exploit the unparalleled ability of integrated microfluidic chips to spatially and temporally control composition within fluids down to the picoliter level to study the kinetics of CO versus oxygen binding to the active site of myoglobin using UV-vis imaging. Presently, chips are being developed and tested in proof-of-principle FTIR imaging experiments designed to characterize biochemical dynamics in the micro- and millisecond time domain.

Cross-Talk between Integrins and Cadherins in Tumorigenesis
P. J. A. Kenis, D. E. Leckband,* J. Silvestre
National Institutes of Health, PHS 1 F31CA126500

Cell-surface and cell-cell receptors have been studied extensively to investigate the switch from benign noninvasive to metastatic tumors. However, one of the major limitations has been the lack of studies that explore the effect of the cellular microenvironment on this transition. In this study we use microfluidic platforms to create gradients of surface-bound extracellular matrix (ECM) and N-/E-cadherin proteins, thereby manipulating the microenvironment that the cell experiences. Cell migration studies on these gradients are elucidating synergies between integrins and cadherins, and thereby increasing our understanding of the effects of the tumor microenvironment and gene expression on metastasis.

* Denotes principal investigator.
**Engineered Platforms to Manipulate Intracellular Redox State**


National Institutes of Health, PHS 1 R21 EB004513

Intracellular redox status exerts influence on the normal cellular processes of DNA synthesis, selective gene expression, cell cycle progression, proliferation, differentiation, and apoptosis. However, molecular mechanisms mediating redox sensitivity are still poorly defined. We have created electrochemical platforms that enable precise manipulation of intracellular redox state. We have also obtained novel genetic constructs that will enable real-time and extended assessment of alterations in intracellular redox without cellular disruption through FRET microscopy. These cell study platforms and biosensors for visualization are now being used to study the relationship between intracellular redox and density-dependent contact inhibition of cell growth, i.e. the role of intracellular redox in uncontrolled cell growth (tumorigenesis).

**High-throughput Stem Cell Isolation and Analysis of the Role of CD34 in Maintaining its Stemness**

P. J. A. Kenis, L. B. Schook, H. R. Gaskins, J. Zhang, T. W. Jensen

Illinois Regenerative Medicine Institute

This multi-investigator project seeks to develop methodologies for isolating stem cells from raw samples and to analyze the potency/properties of the resulting cell fractions. Within this effort, Kenis, Gaskins and coworkers are developing microfluidic platforms for capturing and isolating hematopoietic stem cells (HSCs) from bone marrow or peripheral blood, based on the presence of CD34, a transmembrane protein. In addition, we investigate the role of CD34 in HSCs. CD34 has a cysteine-rich region in its extracellular domain. The presence of three disulphide bonds between the six cysteine residues in this domain suggest potential in regulating redox environment and reducing reactive oxygen species (ROS). This structural information of CD34 can be correlated with the biology of the CD34 positive HSCs. Bone marrow, the home of HSCs, is a hypoxic environment, where the HSCs can be maintained in a reduced condition, which is good for retaining their self-renewal capacity. However, it is unclear how HSCs retain their self-renewing capacity after mobilizing into peripheral blood where they are exposing to a much higher level of oxygen.

**Innovative Methods for Membrane Protein Crystallization**


National Institutes of Health, PHS 1 R21 GM75930

Membrane proteins play key roles in many biological processes and are thus prime targets for intervention in disease-related processes with pharmaceuticals. Unfortunately, the success of crystallization of membrane proteins, necessary for structure determination via x-ray diffraction, lags behind the crystallization of their soluble counterparts due to the amphiphilic nature of membrane proteins. We have created novel microfluidic crystallization platforms and procedures to substantially speed up the process of determining optimal crystallization conditions for membrane as well as soluble proteins. We have shown that precise control of the rate of solvent evaporation (i.e. kinetic control) enables the identification of crystallization conditions for a variety of proteins (e.g., lysozyme, thaumatin, Bacterio-rhodopsin) as well as for the dramatic improvement of crystal quality. Also, we obtained a microfluidic network capable of distributing 48 precipitants in three different protein/precipitant ratios over 144 wells that are each 30 nanoliters in volume. A second microfluidic chip that we developed is able to create lipidic mesophases in sub-30-nanoliter quantities for the crystallization of membrane proteins in a more membrane-like environment. Proof of principle studies with proteins of which the structure is known have been completed, so presently these chips are being applied to the crystallization of proteins whose structure is not known.

**Chemical Imaging of Phase-Separated Lipid Bilayers**

M. L. Kraft, P. Juristyarini, C. R. Anderton

University of Illinois

Compositionally distinct lipid domains within biological membranes, referred to as membrane rafts, are postulated to play important roles in many cellular processes. However, these domains have not been directly observed in cellular membranes, and their precise size and composition have not been established. A better understanding of cell membrane organization can be acquired by studying component mixing in simplified cell membrane models, such as chemically defined supported lipid bilayers, but no general method to quantitatively image the lateral distribution of components in a bilayer exists. We have developed a direct approach for chemical composition analysis of supported lipid bilayers with high lateral resolution: multiple isotope imaging mass spectrometry (MIMS). During MIMS analysis, a focused cesium ion beam is scanned across the sample; the

* Denotes principal investigator.
secondary ions generated by the fragmentation of the surface components are extracted and analyzed according to their respective mass-to-charge ratios at high mass resolving power. By selectively incorporating a unique stable isotope into each membrane component, a component-specific image of the sample can be created. We are currently applying this approach to analyze the component distributions within supported lipid bilayers that contain cholesterol as well as saturated and unsaturated lipids. These studies can have broad implications for our understanding of the molecular interactions that influence lateral heterogeneity within cellular membranes.

Composition Analysis of the Influenza Virus Pre-Envelope by Multiple Isotope Imaging Mass Spectrometry (MIMS)

M. L. Kraft,* K. Lou, W. P. Hanafin
Burroughs Wellcome Fund, Career Award at the Scientific Interface

The influenza virus is hypothesized to assemble and bud at cell membrane domains that are enriched by cholesterol and sphingolipids, but the composition of the pre-envelope membrane domain cannot be analyzed with current methods. We have developed a multiple isotope imaging mass spectrometry (MIMS)-based approach to analyze supported lipid bilayers with lateral resolution. We are extending this methodology to analyze the abundance of cholesterol and sphingolipids at the site of influenza virus budding. Metabolic labeling strategies and antibody labeling schemes are being developed to incorporate distinct atomic labels into the cholesterol, sphingolipids, and influenza virus hemagglutinin within cells. This will allow us to image the secondary ions that are characteristic of the labeled components with MIMS, and to determine whether these components are heterogeneously distributed and co-localized in the membrane. These studies will increase our understanding of how cell membrane organization influences influenza virus replication.

Identification of Cancer Related Membrane Glycans

M. L. Kraft,* Q. Liao, R. L. Wilson
University of Illinois

During cancer progression to metastasis, changes in the structures and distributions of cell membrane glycoconjugates, also called glycans, are observed. Our understanding of the functional roles of these altered glycans would benefit from the development of a method to identify the structures and distributions of glycans in individual cells. We are developing an approach that employs time-of-flight secondary ion mass spectrometry (TOF-SIMS) and multivariate analysis to identify membrane glycans by their mass spectra and image their distributions on individual cells. Successful development of this methodology can lead to a better understanding of the relationship between membrane structure and function within the context of cancer progression.

Cadherin Glycosylation in Oral Cancer

M. Kukurizinska (Boston Univ), D. E. Leckband, M. Langer
National Institutes of Health

Cadherins are essential for development and tissue organization. Their malfunction is also linked to a variety of different cancers. In some oral cancers, cadherins express an unusually high level of carbohydrate modification. However, whether this is the basis of the disease or a consequence has not been established. The goal of this project is to determine the impact of abnormal cadherin glycosylation on cadherin function, and to determine whether these changes alter the cadherin function and thereby contribute to carcinogenesis.

Mechanocoupling at Intercellular Junctions

D. E. Leckband,* N. Wang (Mech. Sci. & Engr.), F. Chowdury, C. Mann, Q. Shi
National Institutes of Health, RO1 GM51338 Reid T. Milner Professorship (Q. Shi)

We are using magnetic twist cytometry and traction force microscopy to determine the molecular mechanisms of transmembrane force transduction and signaling at intercellular junctions. These studies are identifying mechanical components that couple adhesion receptors to the cytoskeleton and enhance adhesive strength through mechano-chemical feedback.

Nanomechanics of Biological Adhesion: from Single Molecules to Tissues

D. E. Leckband,* V. Maruthamuthu, Y.-H. Chien, Q. Shi
National Institutes of Health, RO1 GM51338; Drickamer Graduate Fellowship (VM)

In these studies, we are determining the molecular basis of protein-mediated cell-cell adhesion in tissues. Receptor-mediated cell adhesion is important in wound healing, cancer metastasis, and tissue engineering. This work uses a multiscale approach to establish how the detailed nanomechanics of protein bonds governs the mechanics and formation dynamics of intercellular junctions in tissues. We use a combination of molecular force probe measurements, theoretical modeling, and molecular biology techniques. Our findings are providing critical insights into the connections between protein mutations and human disease.

* Denotes principal investigator.
Smart Materials for Biomedical Applications
National Science Foundation, BES 0349915

This work focuses on the design of biologically active materials for cell culture. This program has two main thrusts. The first is to identify the design parameters that control the interactions of temperature-responsive polymer coatings with biological macromolecules and cells. The second related research objective is to develop novel microfabrication methods for generating tunable, biomaterials with variable mechanical compliance and interfacial properties. These materials will enable the identification of both mechanical and surface properties biomaterials that control cell attachment and function in engineered environments.

Design and Synthesis of Polymeric Materials for DNA Delivery
D. W. Pack,* D. Drake, N. Gabrielson, V. Shum, M. E. Hwang
National Science Foundation, BES-0134163; Siteman Center for Cancer Nanotechnology Excellence; University of Illinois

The goal of this project is to design novel polymers capable of safe and efficient delivery of genetic material to mammalian cells. A first step of this research is to elucidate the structure-function relationships of currently available, off-the-shelf gene-delivery polymers. Thus, researchers are developing quantitative assays that will allow the team to probe the various intracellular barriers to transport of DNA from outside the cell into the nucleus. The resulting structure-function database will provide a basis for intelligent design of new materials with improved safety and efficacy.

Design of Materials for Delivery of Small-Interfering RNA
D. W. Pack,* L. Wong
American Cancer Society

RNA interference is an emerging technology in which small, interfering RNA (siRNA) sequences mediate highly specific shutdown of gene expression. Because many cancers are caused by undesirable expression of a specific gene (an oncogene) or abnormally high expression of a normal gene, RNAi holds the potential to become a new class of anticancer therapy. Safe and efficient delivery of siRNA molecules is the highest hurdle holding back the development of RNAi-based therapies. The goal of this project is to learn how to design polymers to efficiently carry siRNA into tumor cells. The research team investigates how specific properties of polymers control cytoplasmic localization and release of siRNA. The physicochemical properties of polymers and their complexes with siRNA are evaluated, and gene knockdown is investigated in cells growing in culture and in animal models.

Engineering of Viruses for Enhanced Gene Therapy
D. W. Pack,* R. Keswani, D. Drake
National Science Foundation, BES-0602636

The overall goal of this project is to develop a new class of gene delivery vectors by combining “bald” retrovirus-like particles (RVLPs) and synthetic components. RVLPs are essentially intact virions, but lack the viral envelope protein that is responsible for binding to target cells and for virus-cell membrane fusion. RVLPs are therefore noninfectious. Synthetic polycations—polymers or lipids—can electrostatically “complex” with RVLPs to reintroduce cell binding and membrane fusion. In addition, conjugation of appropriate ligands to the synthetic component provides cell-specific targeting. Once inside the cell, the natural virus mechanisms, provided by the RVLP, take over to provide efficient intracellular trafficking and even integration of genes with the host genome providing stable expression. Preliminary results demonstrate the feasibility of hybrid nanovectors for efficient gene delivery. This project is laying a foundation for design and optimization of hybrid vectors, especially for targeted gene therapies.

Nanoparticles for Brain Drug Delivery
D. W. Pack,* S. Anthony
Parkinson's Disease Foundation

The brain is isolated from the systemic circulation by the blood-brain barrier (BBB), formed by the very tight junctions between brain capillary endothelial cells. As a result, most water-soluble drugs, especially macromolecules, cannot be effectively delivered to the brain from the circulation. Safe and effective delivery systems are desperately needed for brain drug delivery, in particular for novel treatments of neurological diseases (e.g., Parkinson’s and Alzheimer’s diseases) and brain cancer. The overall goal of this project is to investigate biodegradable polymer nanoparticles as vehicles for drug delivery to the brain. Nanoparticles are covalently derivatized with targeting ligands that can be transported across the BBB. The team uses both in vitro models of the BBB and in vivo models to investigate the ability of nanoparticles to provide prolonged delivery of drugs to the brain.

* Denotes principal investigator.
**Precision-Release Drug Delivery**  
D. W. Pack,* K. Stovall, K. Smith  
National Institutes of Health

The research team is encapsulating therapeutic compounds in polymer matrices such that the drug can be released at a controlled rate over a prolonged period of time in the body. The approach is unique in that researchers have precise control over particle size, size distribution, and architecture. These characteristics lead to unprecedented control of drug delivery kinetics. Furthermore, the team is pursuing advanced applications, such as passive targeting based on particle size, that have not previously been possible due to the limitations of current fabrication methods.

**Decoding the Secretome for Systems Analysis of Glioblastoma**  
University of Illinois

We are performing a set of fundamental experiments in glioblastoma cell lines to assess the degree to which the secretome can be used to identify causal genetic perturbations and to provide information about the state of biomolecular networks. Specific aims are to generate profiles of the secretome in glioblastoma cell lines for specific siRNA knockdowns and drug treatments to discover the extent to which specific perturbations are reproducibly and uniquely identifiable in the secretome; to generate a predictive genetic regulatory network; and to generate a predictive computational model linking observed patterns in the secretome to likely causal genetic perturbations (or, at a more-coarse level of resolution identify likely perturbed "pathways"). We have initial "proof of concept" of this approach using novel computational methods integrated with a previously available model and data from a model organism, *Halobacterium*. We will study various glioblastoma and glial (noncancerous) cell lines, including the very important subpopulation of cancer stem cells (CD133+), thought to be the primary drivers of tumor growth and regeneration.

**Model-Guided Cellular Engineering of *C. beijerinckii* for Increased Biobutanol Production**  
N. D. Price,* C. Milne, R. Raju, H. Blaschek  
University of Illinois

With the completion of the genome sequence of *C. beijerinckii*, we can now employ the tools of systems biology to gain increased insight into the metabolic and regulatory networks relevant to solvent production.

* Denotes principal investigator.

Transcriptional analysis from Hans Blaschek’s lab using a 500 gene microarray of the *C. beijerinckii* 8052 parent and the hyper-butanol producing BA101 strains during the shift from acidogenesis to solventogenesis revealed significant differences between the two strains with respect to the transcription of genes in multiple functional classes that are necessary for solventogenesis, sporulation, motility, and sugar transport. A systems understanding of these processes will provide the basis for rationale design of this organism in future studies, both in terms of modification beneficial to decreasing the effects of the inhibitors and in terms of maximizing solvent production. A systems approach of particular interest is constraint-based modeling of genome-scale metabolic networks that can be utilized as a basis for interpreting the outcome of experiments and as a basis for metabolic engineering.

**Relative Expression Analysis for Cancer Diagnosis and Prognosis**  
University of Illinois

The assessment of relative expression reversal patterns between phenotypes provides a simple, yet powerful approach to aid in the identification of molecular signatures for disease diagnosis and prognosis. The simplest version of this approach is known as top scoring pair analysis, which we used to identify a relative expression reversal between two transcripts, OBSCN and PRUNE2, that separates two very similar-appearing cancers—gastrointestinal stromal tumor (GIST) and leiomeiosarcoma (LMS)—that require very different treatments (Price et al, PNAS, 2007). We have expanded on this idea with the development of a suite of relative expression analysis methods, including gene set expression ordering index (GSEOI), a novel metric for identifying differentially regulated pathways between sets; gene set expression reversal analysis (GSERA), a new method for comparing sets of high-throughput data based on relationships between a priori defined gene sets (e.g. pathways); relative expression survival analysis (RESA), a method for identifying patterns of marker pairs that aid in cancer prognosis; and relative expression signature translation (REST), which we use to map observed protein signatures to identify likely ranges of states of internal genetic network states.
Bacterial Chemotaxis
C. V. Rao,* K. Wu
University of Illinois

In collaboration with George Ordal (Biochemistry)

Chemotaxis is the process by which cells sense changes in their chemical environment and move toward more favorable conditions. In this research, we are investigating chemotaxis in the Gram-positive bacterium *B. subtilis*. The objective is to understand the molecular mechanisms regulating chemotaxis in this organism and also understand how this pathway evolved in different species of bacteria and archaea.

Quantitative Analysis of Innate Inflammation
C. V. Rao,* P. J. A. Kenis, F. Wang, L. Olson
National Institutes of Health, PHS 1 R01 GM083601

In response to an infection, a body must recruit immune cells to fight off invading microbes. Chemotaxis, the process by which cells move in response to chemical gradients, plays a prominent role in this defense mechanism. A number of chemical signals, called chemoattractants, are produced at or proximal to the site of infection. Immune cells use these chemical signals to target sites of infection and inflammation. Aberrant signaling can delay the immune response, lead to excessive inflammation, or delay wound healing. The objective of this research is to understand how white blood cells use these signals to target microbes during the initial phases of infection. The results of this research will aid in development of anti-inflammatory drugs and vaccine adjuvants.

Regulation of Pentose Transport and Metabolism
C. V. Rao,* T. Desai
Energy Biosciences Institute

Lignocellululose ethanol is a promising alternative to gasoline for future transportation energy needs. The specific problem that we plan to address is multiple sugar utilization. The hydrolysis of lignocellulose yields a sugar mixture consisting mainly of glucose, arabinose, and xylose. *Escherichia coli* can natively metabolize all three sugars. However, multiple sugar utilization in *E. coli* is hampered by so-called "catabolite repression"; the bacterium will always consume just one sugar while repressing the metabolism of all others. We are examining the different factors contributing to catabolite repression and determining their relative roles in establishing the metabolic hierarchy between glucose, arabinose, and xylose.

Reprogramming Transcription and Translation
C. V. Rao,* L. Chubiz, K. Koita
National Science Foundation CAREER

The goal of this research is to develop genetic tools for reprogramming cellular function. To achieve these goals, we are developing new approaches for engineering transcription factors and ribosomes with novel DNA and RNA binding specificity. Such tools will greatly facilitate controlled gene expression and the design of synthetic gene circuits in applications ranging from gene therapy to metabolic engineering. These tools will also be useful for dissecting the native gene circuits controlling cellular physiology.

Salmonella Pathogenesis
C. V. Rao,* S. Saini
University of Illinois

*Salmonella enterica* is a common food-borne pathogen. In the United States, approximately one million nontyphoidal salmonella infections are reported each year, resulting in over ten thousand hospitalizations and one thousand deaths. Worldwide salmonella infections are estimated to cause one million deaths annually. While in most cases salmonella infections can be treated effectively with the use of fluoroquinone antibiotics, the emergence of multidrug-resistant strains indicates that our current portfolio of drugs will become obsolete in the near future. In this research, we are investigating the genetic program used by salmonella during the initial phases of infection. The results from this research will aid in the development of new antibiotics and also provide insights into the general mechanisms of bacterial pathogenesis.

Novel Algorithms for Crystallographic Computing
N. V. Sahinidis*
National Institutes of Health

Since the mid nineteen hundreds, analysis of x-ray diffraction data of crystals has been used extensively for the determination of molecular structure and properties. While the method is employed almost on a routine basis worldwide, it is a major challenge to identify the three-dimensional structure that best fits the diffraction data. A key obstacle, in particular, is the identification of the phases of the diffracted rays from measurements of intensities alone. This problem is known as the "phase problem" in crystallography. We are developing novel combinatorial and global optimization algorithms to resolve this problem.

* Denotes principal investigator.
Implant-Nanofiber Composites Enriched in Bone Marrow-Derived Mesenchymal Stem Cells for Oral and Maxillofacial Rehabilitation

R. Shanti, C. Skotjo,* H. Kong
Osteology Foundation, 07-020

Cell-based tissue engineering is a burgeoning field that aims to integrate principles of engineering and the life sciences to fabricate functional biological substitutes for the restorations of lost or damaged tissues. The integration of novel technologies and principles of tissue engineering to endosseous implants offers an alternative to improve osseointegration. Today, nanofibrous scaffolds are receiving substantial attention as novel biomaterials due to their following properties: morphologically mimic the native extracellular matrix of natural tissues, high surface area to volume ratio, favorable mechanical properties, and wide range of pore size distribution. Bone marrow-derived mesenchymal stem cells offer an additional technology to enhance the process of osseointegration for the following reasons: these cells readily undergo osteogenic differentiation under the appropriate conditions, they are generally considered to be easily accessible and readily available, and they possess extensive self-renewal or expansion capability. We hypothesize that by coating the implant surface with an artificial milieu that mimics the native extracellular environment enriched in cells with tremendous regenerative potential will significantly enhance the process of osseointegration.

Near IR Signal Transduction of Molecular Binding to Single Walled Carbon Nanotube Biosensors

M. S. Strano,* P. Barone, D. Heller, E. Jeng, C. Y. Lee
National Science Foundation; Mattek Corp.

Near infrared light can penetrate thick tissue and whole blood samples forming the basis of in vivo sensing technologies. However, few organic molecules emit in this region in a stable manner. Carbon nanotubes hold particular advantage as sensor elements because their 1-D electronic structure renders carrier transport more sensitive to scattering from adsorbates than from intrinsic mechanisms. We are designing nanotube systems that act as optical biosensors that respond to analyte binding at tailored receptor locations with a modulation in near infrared optical response. Such sensors are ideal for implantation into human tissue to provide real time information about biochemical concentrations in a noninvasive manner.

Biomolecular Engineering via Directed Evolution

H. Zhao,* M. McLachlan, V. Gonzalez
National Science Foundation CAREER

The team is interested in developing a novel receptor-based gene expression system in which activity can be precisely regulated by a synthetic ligand. We will use a combined rational design and directed evolution approach to engineer a fully orthogonal ligand–receptor pair consisting of an estradiol derived synthetic ligand and a human estrogen receptor ligand binding domain mutant. Such a system is an invaluable tool for gene therapy, temporal control of the onset of phenotypes in transgenic animals, regulated expression of genes in plants, and biological study of development and other physiological processes.

Directed Evolution of Metalloenzymes for Organic Synthesis

H. Zhao,* H. Lu
National Science Foundation CAREER

In collaboration with the research group of John Hartwig (Chemistry)

Directed evolution has become a proven method for the development of enzymes that display non-natural functions. The team is interested in developing metalloenzyme based selective oxidations for reactions useful in organic synthesis and selective halogenations that provide building blocks for medicinal chemistry.

Directed Evolution of Novel Homing Endonucleases for Gene Therapy

H. Zhao,* F. Wen, N. Sun, Y. Nakagawa
National Institutes of Health; OMT, Inc.

Gene therapy has the potential to significantly influence human health in this millennium and promises new treatment for a large number of inherited and acquired diseases. However, due to the difficulties in achieving sustained gene expression and in safe and efficient gene delivery, gene therapy has been of limited medical benefit. To address these limitations, the proposed research will seek to develop a novel technology based on engineered homing endonucleases that enables correction of diseased genes in mammalian cells, with particular application to sickle cell anemia.

* Denotes principal investigator.
**Discovery, Design, and Development of Phosphonic Acid Antibiotics**

H. Zhao,* T. Johannes, Z. Shao, C. Denard, N. Nair  
*National Institutes of Health*

*In collaboration with research groups of William Metcalf (Microbiology), Wilfred van der Donk and Neil Kelleher (Chemistry), and Satish Nair (Biochemistry)*

Phosphonic acids represent a potent, yet underexploited, group of bioactive compounds with great promise in the treatment of human diseases. The team is interested in characterizing and engineering two specific phosphonic acid antibiotics, fosfomycin (an FDA-approved antibiotic) and FR900098 (an antimalarial agent). Both protein engineering and metabolic engineering approaches are used in combination with a wide variety of biochemical and biophysical methods.

**Engineering a Yeast Strain that Efficiently Utilizes C5/C6 Sugars**

H. Zhao,* J. Du, R. Sullivan  
*BP Energy Biosciences Institute*

Fermentative conversion of renewable, inexpensive lignocellulosic biomass to biofuels such as ethanol and butanol could meet a large portion of this nation’s demand for transportation fuel. And the fermentation of almost all the available C6 and C5 sugars to ethanol or other liquid biofuel is vital to the overall economics of these processes because this will maximize the yield and minimize the costs associated with waste disposal. The researchers are engineering a yeast strain capable of efficiently utilizing C5/C6 sugars for the economical production of biofuels. The ultimate goal of the project is to design a recombinant yeast that will pass the target set in the 2006 DOE bioethanol roadmap in terms of sugar utilization, i.e. use of C5/C6 sugars to produce ethanol with yield greater than 95% of theoretical maximum.

**Computing**

**Supercomputing Studies of Wall Turbulence**

T. J. Hanratty,* Y. Mito  
*Grant, University of Illinois College of Liberal Arts and Sciences*

We are studying the structure of turbulence and are exploring new methods of interpreting turbulent transport of molecular species or particles that describe the field as resulting from a distribution of sources and sinks. These studies are carried out with a supercomputer simulation of turbulent flow in a channel and are made possible by the development of particle tracking routines. Of particular interest is the influence of particles on fluid turbulence.

**Fluid Flow, Heat, and Mass Transfer Fundamentals**

**Gas-Liquid Flows**

T. J. Hanratty,* Y. Mito  
*Grant, University of Illinois College of Liberal Arts and Sciences*

The goal of this work was to relate the distribution of the phases to small-scale interaction. Stochastic methods are being explored to describe droplet dispersion and deposition in annular flows.

**Computational Study of Three Dimensional Concentrated Emulsions with Surfactant Effects**

J. J. L. Higdon,* K. Higa  
*National Science Foundation*

Multiphase fluid flows are encountered in a wide array of industrial operations in the petroleum, chemical, food processing, personal care products, and other industries. Surfactants are nearly omnipresent in all industrial processes involving multiphase fluids. These agents are added to optimize the processing conditions: stabilizing or destabilizing the multiphase fluid; adjusting its viscosity, elasticity or yield stress; modifying droplet size or size distribution; or affecting numerous other properties specific to a given product or industry. Large-scale, three-dimensional multiphase flow simulations are being developed for highly concentrated emulsions and foams. The flow analysis will focus on three thrusts: to characterize the rheology and phase behavior of the suspensions in linear shear flows; to analyze surfactant transport and the microscale mechanisms through which the surfactants modify suspension behavior; and to analyze the multiphase fluid flow through three dimensional model porous media. Detailed comparisons of experiments and simulations will be conducted.

**Direct Numerical Simulation of Microscale Rheology and Multiphase Flow in Porous Media**

J. J. L. Higdon,* A. Kumar  
*ACS, Petroleum Research Fund*

Multiphase fluid flows are encountered in enhanced oil recovery operations and in manufacturing operations in the petrochemical industry. This research utilizes large-scale, three-dimensional hydrodynamic simulations to study highly concentrated emulsions and foams. A new computational approach is implemented combining a

* Denotes principal investigator.

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**Notes:**
- * indicates principal investigator.
spectral boundary integral method with the PME (particle mesh Ewald) approach. The research will focus on two distinct thrusts: to characterize the rheology and phase behavior of the suspensions in linear shear flows, and to analyze the multiphase transport through three-dimensional model porous media. For the transport in porous media, attention will focus on the relative distribution and transport of the two phases and the effect of pore-constriction geometries on transport properties.

Mechanics of Suspensions
J. J. L. Higdon,* K. Higa, M. Bybee, A. Kumar
Mobil Corporation; U.S. Department of Energy

Concentrated suspensions of microscopic particles are encountered throughout the chemical process industry. The goal of this project is to characterize the rheology and sedimentation behavior of these systems, with special attention given to suspensions with nonhydrodynamic interparticle forces and particles of nonspherical shape, such as fibers and platelets. Researchers are developing novel computational algorithms for large-scale, many-body simulations to investigate these systems. The methods follow the basic approach of the well-known Stokesian dynamics algorithm, but yield an operational count $O(N)$ as opposed to the $O(N^3)$ effort of the traditional approach.

Effect of Free Polymer on Protein Interaction Potentials
C. F. Zukoski,* A. Bonner, A. Mirarefi
National Aeronautics and Space Administration, NAG 8-976

Protein crystals are often produced through the addition of soluble polymers to protein suspensions. In this study, the effects of polymer molecular weight and concentration on the strength of protein interactions are investigated. An unexpected minimum in protein solution second virial coefficient is observed. This phenomenon is intimately related to polymer depletion forces and polymer density fluctuations resulting from the proximity of a polymer solution phase boundary.

Materials

Multiscale Simulations of Electrochemical Systems
R. C. Alkire,* L. Petzold, R. Braatz
National Science Foundation; National Resource Allocation Committee, MCA00N016

The physical applications of interest include electrodeposition of copper and degradation of industrially significant metals by corrosion. Numerical simulations of these applications involve phenomena that span over 10 orders of magnitude of scale in time and distance. The computational resources support deterministic (continuum) as well as stochastic (noncontinuum) methods separately and, by linking them, enable multiscale investigations of deposition and dissolution processes.

Improved Metal Catalysts with Properties Controlled by Semiconductor Band Engineering
E. G. Seebauer,* S. Ong, M. Kratzer
Singapore A*STAR, University of Illinois at Urbana-Champaign Partnership Program

Catalysts with metals on semiconducting oxides have proven to be quite useful for applications in fuel cell cathodes and hydrogen production. This project seeks to employ principles routinely used in the design of nanoscale integrated circuits to circumvent these problems. Such devices often use “heterojunctions,” which are structures in which two different kinds of semiconductors are sandwiched together. Such heterojunctions form the basis of laser pointers, but we believe the same principles can be employed with oxides of metals such as titanium, zinc, and iron to make “catalyst heterostructure” devices. In particular, this work seeks to employ principles of semiconductor band engineering to deliberately control the electronic structure of metals in compound catalysts. An entirely new class of catalysts is being created, in which nanoscopically thick layers of metal are deposited atop semiconductor substrates. The substrate type and doping level will be chosen to tune the surface properties of the metal by the “Schwab effect.” Quantum calculations by density functional theory will be used to help predict the type of semiconductor and doping to use for the substrate, as well as the thickness of the metal required. The requisite structures will then be created by deposition methods drawn from microelectronics processing, and the properties of the semiconductor-metal catalysts will be characterized by optical and electron-based methods.

Improved Photocatalysts with Properties Controlled by Semiconductor Band Engineering
E. G. Seebauer,* M. Kratzer
National Science Foundation, DMR 07-04354

The microelectronics industry has developed principles for the design of metal/semiconductor structures to obtain novel and controllable electrical behavior in integrated circuits. Many of these principles should be adaptable to obtain novel and controllable chemical behavior in catalysts. This work seeks to demonstrate how to employ the notion of electronic band engineering in
semiconductors to create an entirely new class of catalysts with controllable properties. Since metal oxide catalysts are semiconductors that can support electrical charge distributed in space, it is possible for surface electronic properties to couple to bulk electronic properties. We believe the electronic band structure of the underlying support can be tailored to beneficially affect the electronic properties (average charge state, reducibility, and so forth) of the free surface. Successful demonstration of such structures would have broad applications in environmental photocatalysis by TiO$_2$.

**Measurement of Illumination Induced Diffusion in Oxide Semiconductors**  
E. G. Seebauer,* R. Vaidyanathan  
*Applied Materials*

The present work seeks to develop entirely new forms of defect manipulation in oxide semiconductors, such as titanium dioxide, based on optical stimulation of defect formation and migration. Diffusion measurements have shown that defect mobilities and concentrations can be nonthermally modulated in semiconductors by super-band gap illumination. Specially synthesized structures are used to measure motion of vacancies and interstitial atoms. Quantification is accomplished through detailed continuum modeling backed by characterization of near-surface electric fields through optical photoreflectance.

**New Methods for Defect Manipulation in Semiconducting Oxides**  
E. G. Seebauer,* A. Hollister  
*National Science Foundation, DMR 07-04354*

Through experiments and modeling, we seek to develop entirely new forms of defect manipulation in oxide semiconductors using surfaces. Solid-state diffusion measurements have quantified how surfaces react with bulk point defects such as interstitial atoms and vacancies. The chemistry is comparable in richness to the reactions of surfaces with gases. Up to now, little attention has been paid to this alternative form of surface chemistry, even though it can play a primary role in regulating bulk defect concentrations. In semiconductors, bulk-surface coupling occurs through electrostatic and surface bond insertion/generation mechanisms. The science base to be developed here should offer entirely new possibilities for controlling bulk defects in a wide variety of applications. Such defect manipulation might also be helpful for energy production by semiconductors using solar power (e.g., water splitting), where electron-hole recombination rates in the fabricated devices are affected by the concentrations of bulk defects left over from device fabrication.

**Multifunctional Nanocomposites Based on Single Walled Carbon Nanotubes**  
M. S. Strano,* R. Graff, J. Swanson  
*United States Air Force*

Carbon nanotubes are the strongest molecular fibers realized to date. Single nanotube tensile strengths exceed 1 TPa. Our interest is in the synthesis of ultra-strong composites with multiple functionalities, such as embedded electronics, electromagnetic absorption for shielding, and electromechanical modulation. To accomplish this, nanotubes need to be dispersed into a matrix at the single molecule level. We are developing new fabrication techniques that allow unprecedented control of nanoscale interfaces for the next generation of “smart” materials.

**Using 1-D Electron Transfer Chemistry to Control Field Effect Transistor Performance for Flexible-Electronic Applications**  
M. S. Strano, M. Usrey, C. Y. Lee, M. Alexander, J. Rogers*  
*Defense Advanced Research Projects Agency*

Single walled carbon nanotubes have electron mobility far in excess of known materials (700,000 cm$^2$/Vs) and hence are ideal for nano electronic applications. Flexible circuits and displays are desirable as the basis for new technologies including electronic paper, transportable sensors, robust computer processors and wearable flat panel display projections. Semiconducting carbon nanotubes can operate as field effect transistors for such applications, but metallic impurities short circuit carrier transport and prevent discrete switching. This project seeks to apply knowledge regarding charge transfer to 1-D nanotube systems to selectively rupture carbon bonds of impurity pathways. We seek to map device improvement in terms of on-off ratios to specific chemical pathways, thus providing a useful handle for nano electronic control.

**Assembly of Nanoparticles**  
C. F. Zukoski,* E. Mock  
*U.S. Department of Energy, DEFG02-91ER45439*

*In cooperation with the Frederick Seitz Materials Research Laboratory*

Particles with anisotropic interactions are synthesized and used to assemble novel microstructures. Using novel synthesis techniques we control the physical and chemical anisotropy of particles, with the goal of studying how anisotropy affects microstructural arrangements. Links between particle microstructure and macroscopic optical and rheological properties are studied. We are interested in

* Denotes principal investigator.
how anisotropy can be used to engineer novel complex particle arrangements.

**Characterization of a Strongly Aggregated Model Gel System**

C. F. Zukoski,* R. Kramb  
*U.S. Department of Energy, DEFG02-91ER45439  

In cooperation with the Frederick Seitz Materials Research Laboratory

A model gel system has been developed in which the dominant force of attraction is van der Waals forces. In this system, solutions of colloidal spheres with diameters from 200nm to 1μm are coated with a nonionic surfactant. The particles aggregate to form gels as the background ionic strength is raised and electrostatic repulsion is screened out. Accurate predictions of strength and range of interparticle attractions are sought using characterization methods including: finding the ionic strength-volume fraction gel line, measuring mechanical properties both near the gel point and deep within the gel, and determining microstructure using light and neutron scattering techniques.

**Flow of Weakly Flocculated Suspensions**

C. F. Zukoski,* S. J. Yoon  
*U.S. Department of Energy, DEFG02-91ER45439  

In cooperation with the Frederick Seitz Materials Research Laboratory

In this investigation, researchers examine the flow properties of weakly flocculated suspensions. A model system has been chosen in which, by solution pH, the suspension can be reversibly gelled. By mapping out a phase boundary in pH/volume fraction space, the research team is able to explore the relationship between flocculation in colloidal suspensions and sol-gel transitions observed in molecular systems. The mechanical properties of the gelled samples are of importance in determining porosity and suspension processibility. Researchers are seeking general descriptions of yielding and flow in terms of the depth of the interparticle attractive potential.

**Microstructure and Mechanics of Filled Polymer Melts**

C. F. Zukoski,* B. J. Anderson  
*Nanoscale Science and Engineering Initiative of the National Science Foundation, NSF Award No. DMR-0117792

We explore the effects of polymer molecular weight, nanoparticle volume fraction, and polymer-particle surface affinity on the microstructure and mechanics of filled polymer melts. The design of these materials is often hindered by inadequate particle dispersion resulting in low product performance. Thus, these studies are conducted to understand the stability and behavior of nanoparticles dispersed in high molecular weight solvents. A variety of phases are expected as molecular weight, volume fraction and surface affinity are varied: homogeneous fluid, phase separation, or nonequilibrium gel. Materials are characterized through scattering and rheological techniques.

**Microchemical, Microfluidic, and Nanochemical Systems**

**Cathode Catalysis for Hydrogen/Oxygen Fuel Cells**

*Department of Energy, DE-FG02-05ER46260

In hydrogen-based proton electrolyte membrane fuel cells (PEMFCs), the Nafion membrane separates the anodic and cathodic compartments of fuel cells. The cathode typically limits the cell’s performance due to poor kinetics of the oxygen reduction reaction. In addition, flooding of the cathode often occurs, hampering oxygen in trying to reach the cathode. We have developed a microfluidic hydrogen-oxygen fuel cell with a flowing electrolyte between two gas-diffusion electrodes. This electrolyte stream effectively removes excess water from the cathode side, thus eliminating cathode flooding. A reference electrode in the outlet stream allows for independent analysis of the polarization losses on the anode and the cathode, thereby creating an elegant catalyst characterization and optimization tool. We studied the performance of different catalyst ink compositions on the cathode side, including various nonplatinum based catalysts (e.g. Ag nanoparticles). This microfluidic fuel cell lends itself also for operation in alkaline media, which is known to enhance reaction kinetics.

**Distributed Nano Fuel Cells Compatible with Transistor Fabrication**

P. J. A. Kenis,* P. O. Lopez-Montesinos  
*Grainger Emerging Technologies Program

Most present fuel cell technologies use polymer electrolyte membranes such as Nafion to separate the anode and cathode compartments. While these fuel cell technologies hold promise to replace other power sources, most notably batteries, their introduction to the market has been seriously hampered by issues related to these membranes, most notably fuel crossover, catalyst leaching, anode dry-out, and cathode flooding, all leading to reduced...
performance. Here, we develop silicon-based microfuel cells in which the membrane has been replaced with microfabricated structures, such that it can be fabricated side-by-side with electronic elements, and thus implemented in distributed fashion within electronic architectures.

**Electrostatic Valves for Integrated Microfluidics**  
P. J. A. Kenis,* J. Tice, S. L. Perry  
*DOE, Sandia National Laboratory, LDRD PR#922327*

Present microfluidic technology to create highly integrated, large-scale microfluidic networks typically relies on pneumatic pumps and valves for driving and routing fluid flow. This approach requires a lot of chip connections as well as a bulky, external pneumatic control system that needs a source of pressure (i.e. vacuum or compressed air). To overcome these limitations of pneumatic controls, we pursue the development of highly scalable electrostatic valves for large-scale microfluidic chip technology. The electrodes needed to create these valves require minimal space within the chip, and can be controlled using much smaller electronic peripherals. The resulting microfluidic networks will be applied in chips for crystallization purposes and microanalysis applications.

**Membraneless Microfuel Cells**  
P. J. A. Kenis,* R. S. Jayashree, F. R. Brushett, A. Hollinger  
*National Science Foundation, CTS 05-47617 CAREER Award; Northrop Grumman Space Technology*

In most microscale fuel cells, a proton electrolyte membrane (PEM) separates the anodic and cathodic compartments. Fuel crossover and water management issues (cathode flooding, anode dry out) are the main problems in PEM-related fuel cells. In the membraneless laminar flow fuel cells (LFFCs) studied here, the fuel and oxidant stream are brought together in a channel of microscopic dimensions and continue to flow laminarly in parallel without turbulent mixing while the fuel and oxidant can react at the anode and cathode, respectively, placed on opposite sidewalls. Fuel crossover and water management issues can be minimized in this design by fine-tuning the flow rates and channel dimensions. We optimized the performance of air-breathing LFFCs that are fuel flexible (methanol, formic acid) and media flexible (acidic, alkaline) by the combination of results from simulation (three-dimensional finite-element-method) and experiment. We investigated the impact of different operating conditions (volumetric flow rate, fuel to electrolyte flow rate ratio, oxygen concentration) and of different cell dimensions (electrode-to-electrode distances, channel length) on the maximum power density of individual LFFCs. Fuel utilization in a single pass was improved by hydrodynamic focusing of the fuel as a thin stream on the anode to reduce the fraction of fuel that passes through the channel without reacting. Similarly, we exploited the concept of media flexibility to create bio-LFFCs, where the anode and the cathode operate at different pHs and enzymes were used as anode catalysts.

**Microscale Approaches to Pharmaceutical Crystallization**  
*ICES, A*Star, Singapore*

Pharmaceuticals are often manufactured as microcrystals, ideally in the most stable polymorph. We have shown the selective, direct crystallization of the gamma polymorph of glycine, a well-known model compound for polymorphism of pharmaceuticals, in an evaporation-based crystallization platform that enabled kinetic control over the process. In addition, we are developing microfluidic methods to identify all possible polymorphs of novel pharmaceuticals, and to identify the most robust crystallization procedures for the selective crystallization of the thermodynamically most stable polymorph, for example as a salt. Efforts are also under way to study the complex phase behavior of cocrystals, given their emerging relevance and utility in the formulation of pharmaceuticals.

**Microscale Systems for Nanomanufacturing**  
*National Science Foundation, DMI 03-28162, Nanoscale Science and Engineering Center (NSEC)*

The overall goal of Nano-CEMMS, the National Science Foundation NSEC grant here at Illinois, is the development of fluidic and ionic-based nanomanufacturing technology. We identified the critical parameters that determine the amount of fluid (e.g. ink) transferred from one surface to the next for substrates of different hydrophilicity. Subsequently, we used this knowledge to print droplets as small as 70 femtoliter in a two-step procedure starting from microliter-sized droplets. We also created multiplexed arrays of electric sensors (resistive, capacitive, conductive) to track plugs of fluid (e.g. ink) through a microfluidic network, enabling feedback control of these plugs being routed to a certain nozzle in a multinozzle nanomanufacturing toolbit. The multiplexing concept dramatically reduces the number of leads required to monitor events in an mxn sensor array, specifically from

* Denotes principal investigator.
2m×n to m+n+1, so for a 10×10 array, from 200 to 21 leads. In addition, we integrated novel microfluidic networks comprised of nanoliter-sized wells with photonic crystal-based biosensors for the combinatorial synthesis and screening of drug leads (with B. Cunningham). Part of the latter effort is the successful development of actuate-to-open valves that are closed in rest, highly desirable for experiments that take a long time. Presently we are pursuing the manufacturing of fully integrated microfluidic chips for multinozzle manufacturing toolbits through heterogeneous integration and transfer printing approaches.

**Catalysts for Water Treatment**

R. I. Masel,* N. Ndiege

*Center of Advanced Materials for the Purification of Water with Systems (WaterCAMPWS) through National Science Foundation, CTS 01-20978*

The objective of this project is to examine novel photocatalysts for water treatment.

**Fuel Cells for Portable Power**


*Defense Advanced Research Projects Office, DST 200700299513-000*

The objective of this project is to develop novel fuel cell systems for micropower generation. Parts of the work include developing formic acid fuel cells for micropower generation, catalyst development, construction and testing of silicon fuel cells, development of novel membrane materials, and spectroscopic investigations to understand how micropower systems are different than systems on the macroscale.

**Micro-Gas Chromatographs**


*Defense Advanced Research Projects Agency, FA8650-04-1-7121; United States Air Force*

The objective of this project is to construct chip-scale gas chromatographs for hazardous gas detection. The work includes developing MEMS pumps and valves for gas sampling and flow control; a fast preconcentration technology using silicon nanograss and selective adsorbents to suppress unwanted species; a fast, ultrahigh resolution, separation technology using high-aspect ratio DRIE columns and nanoengineered stationary phases; microscale thermal isolation using components suspended on polyimide films; and a three-mode orthogonal micro detection system.

**Microreactors for Hydrogen Production**

R. I. Masel,* M. A. Shannon,* V. Subramanian, L. Zhu

*Defense Advanced Research Projects Office, DST 200700299513-000*

Microreactors are being designed and built to produce hydrogen for small-scale fuel cells using novel chemistries and nanofluidic control systems.

**Multiscale Systems**

**Computational Toolbox for the Investigation of Multiscale Surface Processes**

R. C. Alkire, L. Petzold,* T. Yang (Univ. of California, Santa Barbara), R. Stephens

*National Science Foundation, ITR 04-28912*

The physical system under study is electrodeposition of metallic nanoclusters with use of additives to achieve specific shapes. Key issues are to understand how small-scale surface interactions guide spontaneous self-organization, how to extract insight from noisy data and uncertain fundamental understanding, and how to ensure quality control at multiple scales in manufacturing. The algorithms and software developed for multiscale simulation and sensitivity analysis are generic over a broad class of problems and will contribute well beyond the applications used in their development.

**Analysis and Design of Multiscale Simulation Codes**

R. D. Braatz,* R. C. Alkire,* R. Stephens

*Intel; National Science Foundation, NRAC MCA 01S022, DGE-0338215*

Chemical reacting systems involve phenomena that span several orders of magnitude in time and length scales, from the molecular to the macroscopic. Many papers have adopted a simulation architecture that employs dynamically coupled simulation codes, in which each code simulates the physicochemical phenomena for a different range of length scales in the reacting system. We use nonlinear systems theory to design coupling algorithms that modify the dynamic information passed between stochastic and deterministic codes to numerically stabilize their coupling and increase the numerical accuracy of the simulation results. The methods have been used to guide the design of a multiscale simulation code for copper electrodeposition, which is the process used to manufacture the submicron interconnects in various

* Denotes principal investigator.
The multiscale simulation couples a (2+1)-dimensional kinetic Monte Carlo simulation code that tracks the motion of molecules on the copper surface with a level set code that tracks the position of the moving solid-liquid interface and a finite volume code that simulates the diffusion and migration of chemical species in the electrochemical solution.

Optimization and Process Systems Engineering

Branch-and-Reduce Algorithms for Global Optimization
N. V. Sahinidis*
ExxonMobil Upstream Research Company

Realistic treatments of physical and engineering systems frequently involve nonlinear models in which optimization requires escaping from local minima traps. This project develops global optimization methodologies. The algorithms solve sequences of convex underestimating subproblems obtained by evolutionary subdivision of the search region. Novel features include optimally based and feasibility based range reduction, new branching rules, new bounding schemes, and efficient heuristics to accelerate convergence. The project addresses applications in engineering design, molecular structure determination, and economics. Special classes of problems are also considered, including minimization of concave functions over convex sets, minimization of products of convex functions, bilinear programs, integer programs, and factorable programs.

Processing

Experiments for Control of Transient-Enhanced Diffusion in Transistor Fabrication
E. G. Seebauer,* S. H. Yeong,
M. P. Srinivasan (Natl. Univ. of Singapore),
B. Colombeau (Chartered Semiconductor),
L. Chan (Chartered Semiconductor)
Chartered Semiconductor Manufacturing

Formation of extremely shallow pn junctions with very low electrical resistance is a major stumbling block to the continued down scaling of microelectronic devices. Recent work in our laboratory has shown that the behavior of defects within silicon can be changed significantly by controlling the chemical state at the surface. Certain chemical treatments of the surface induce it to act as an active “sink” for point defects that removes Si interstitials selectively over impurity interstitials, leading to less dopant diffusion and better electrical activation. The present work demonstrates such effects experimentally for several dopants such as boron, arsenic, and phosphorous in both crystalline and Ge pre-amorphized silicon wafers. Moreover, such active surfaces dramatically reduce the number of end-of-range defects observed after annealing.

Modeling for Control of Transient-Enhanced Diffusion in Transistor Fabrication
E. G. Seebauer,* R. D. Braatz, C. T. M. Kwok
American Chemical Society Petroleum Research Fund, 43651-AC5

Transient-enhanced diffusion (TED) during annealing after ion implantation limits how the shallow junctions can be made in next-generation transistors. Models for TED in current commercial process simulation software do not incorporate surface effects adequately. We are incorporating these new aspects of physics through systems-based methods such as Maximum Likelihood estimation and Maximum A Posteriori estimation, and testing the results experimentally in the ion implantation of boron into silicon. Two-dimensional simulations based on this model indicate that the beneficial effects of active surfaces in the source-drain region extend laterally to the surface toward the channel region of a device as well as perpendicularly to the surface into the bulk.

Separation of Single Walled Carbon Nanotubes According to Electronic and Geometric Structure
M. S. Strano,* M. Usrey, D. Heller
Dupont; Ocean Optics Inc.

Carbon nanotubes are a diverse class of electronic and optical materials. Depending on their diameter and helical twisting, nanotubes can be metallic, semimetallic or semiconducting. All currently known synthesis methods create random mixtures of all types, but to use these materials as nanoelectronic circuits and sensors, one needs to isolate and control one particular type. We are developing robust methods to sort and separate carbon nanotubes into distinct fractions for electronic applications.

* Denotes principal investigator.
Control of Crystal Size and Shape Distribution in Pharmaceutical Crystallization
National Science Foundation, ESI-0426328; Eli Lilly

Most pharmaceutical compounds are produced in crystalline form. An integrated approach is being created to control pharmaceutical crystallization that incorporates first-principles simulation models, optimization theory, nonlinear feedback control, and state-of-the-art analysis. This includes simulating the nucleation, growth, and aggregation of crystals with multiple characteristic length scales, designing algorithms for constructing crystal size and shape distributions from in situ video microscopy and laser backscattering, analyzing the sensitivity of the states and product quality variables to model uncertainties, and designing algorithms to control the properties of the product crystals.

Economic Design of Maintenance Policies for Deteriorating Systems
R. D. Braatz,* J. Isom
United Technologies Corporation Fuel Cells

When an alarm is used to initiate an action on a stochastically deteriorating system, the economic impact of a maintenance policy can be assessed with a reliability model, cost model, and process model of the stochastic system. We are developing Markov Chain methods for the design of optimal maintenance policies. Direct search over subsets of the measurement space is practicable only in simple cases. Search of the feasible stopping probability boundary yields optimal results through global minimization. The likelihood ratio method solves a simpler minimization to produce results that are nearly globally optimal.

Journal Articles

Biochemical and Biomedical Engineering


* Denotes principal investigator.


**Fluid Flow, Heat, and Mass Transfer Fundamentals**


**Microchemical, Microfluidic, and Nanochemical Systems**


**Optimization and Process Systems Engineering**


**Systems and Control**


**Book Chapters**

**Systems and Control**


**Papers Presented at Conferences and Symposia**

**Biochemical and Biomedical Engineering**

Desai, T. and Rao, C. V. Engineering transcription factors with novel DNA-binding specificity. 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).

Drake, D. M. and Pack, D. W.  
**Biochemical investigation of intracellular transport of polyethylenimine/DNA polyplexes.**  
Fluid Flow, Heat, and Mass Transfer Fundamentals


Bybee, M. D. and Higdon, J. J. *Phase behavior and microstructure for colloidal systems with attractive/repulsive interparticle potentials*. 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).


Materials


Microchemical, Microfluidic, and Nanochemical Systems


Bhamidi, V., Kenis, P. J., and Zukoski, C. F. *Influencing polymorph selectivity through antisolvent crystallization in microfluidic channels*. 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).

Bhamidi, V., Talreja, S., He, G., Kenis, P. J., and Zukoski, C. F. *Estimation of nucleation kinetics from the kinetic limit of metastable zone width*. 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).

Bhamidi, V., Talreja, S., He, G., Kenis, P. J., and Zukoski, C. F. *Kinetic limit of metastability in crystal nucleation from solution*. 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).


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Gupta, C., Shannon, M. A., and Kenis, P. J. **Analysis of charge transport and associated surface charge densities in thin-film modified electrodes.** 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).


Haan, J. L. and Masel, R. I. **Enhancement of the oxidation of formic acid on palladium and platinum blacks by an increase in the formic acid pH.** 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).

Haan, J. L., Dunbar, Z., and Masel, R. I. **An increased activity for the direct formic acid fuel cell by the addition of metal adatoms to the palladium black anode catalyst.** 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).

He, G., Tan, R. B. H., Kenis, P. J., and Zukoski, C. F. **Generalized phase diagram and metastable states of molecular solutions.** 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).


Kapoor, A., Caporali, E., Stewart, M. C., and Kenis, P. J. **Micropatterned surfaces to control the alignment and proliferation of tenocytes.** 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).

Karulkar, M., Alkire, R. C., and Braatz, R. D. **Simulation of copper nucleation on gold: Investigating the effects of additives.** 211th Meeting of the Electrochemical Society (Chicago, IL, 8 2007).

Kenis, P. J. **Ceramic microreactors for reforming of hydrocarbons.** 9th International Conference on Small Fuel Cells for Portable Applications (Miami, FL, Mar. 2007).


Kenis, P. J. **Microfluidic platforms for membrane protein crystallization.** National Institutes of Health Roadmap Meeting (San Diego, CA, Nov. 2007).

Kenis, P. J. **Microscale approaches to address challenges in energy and biology.** David Reinhoudt Retirement Symposium (Enschede, Netherlands, Sep. 2007).


Kenis, P. J. **Microscale systems: Applications in energy and biology.** 5th International Workshop on Micro Chemical Plants (Osaka, Japan, Jan. 2007).

Kenis, P. J., Jayashree, R. S., Zhou, W. P., and Brushett, F. **Fuel and media flexible microfluidic fuel cells.** 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).


Kenis, P. J., Perry, S. L., Tice, J. D., and Roberts, G. W. **Microfluidic platforms for membrane protein crystallization.** 2007 American Crystallographic Association Meeting (Salt Lake City, UT, Jul. 2007).


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Radadia, A. D., Shannon, M. A., and Masel, R. I. Dispersion effects of microchannel configurations on microGC performance. 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).

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Ranga, J. S., Mitchell, M., Natarajan, D., Markoski, L., and Kenis, P. J. Hydrogen fuel cells with flowing sulfuric acid as the electrolyte. 211th Meeting of the Electrochemical Society (Chicago, IL, May 2007).

Schudel, B., Choi, C., Toepke, M., Cunningham, B. T., and Kenis, P. J. **Combinatorial chemistry chips with photonic crystal biosensors.** 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).

Spendelow, J., Goodpaster, J., Kenis, P. J., and Wieckowski, A. **Methanol oxidation on Pt(111)/Ru in alkaline media.** 212th Meeting of the Electrochemical Society (Washington, DC, Oct. 2007).


Zhou, W., Jayashree, R. S., Brushett, F., and Kenis, P. J. **Characterization of non-Pt based cathodes in an alkaline microfluidic H$_2$O$_2$ fuel cell.** 212th Meeting of the Electrochemical Society (Washington, DC, Oct. 2007).

**Optimization and Process Systems Engineering**

Bao, X. and Sahinidis, N. V. **Automatic convexity detection for global optimization.** 2nd International Conference on Continuous Optimization (Hamilton, ON, Aug. 2007).

Bao, X. and Sahinidis, N. V. **Automatic convexity detection for global optimization.** 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).


Rios, L. M. and Sahinidis, N. V. **Comparison of derivative-free optimization implementations of deterministic computer experiments.** 2nd International Conference on Continuous Optimization (Hamilton, ON, Aug. 2007).


**Processing**


Systems and Control


Kee, N., Tan, R. B. H., and Braatz, R. D.  **Selective crystallization of the metastable anhydrate form in the enantiotropic pseudo-dimorph system of L-phenylalanine using feedback concentration control.** 2007 American Institute of Chemical Engineers Annual Meeting (Salt Lake City, UT, Nov. 2007).

**Theses**

**Biochemical and Biomedical Engineering**


**Fluid Flow, Heat, and Mass Transfer Fundamentals**


**Materials**


**Microchemical, Microfluidic, and Nanochemical Systems**


**Multiscale Systems**


**Optimization and Process Systems Engineering**

Systems and Control


Patents

Materials


Microchemical, Microfluidic, and Nanochemical Systems


Awards and Honors

Richard C. Alkire
Member, National Academy of Engineering
Fellow, American Association for the Advancement of Science
Fellow, Honorary Member, and Past President, The Electrochemical Society
Teaching Excellence Award, University of Illinois School of Chemical Sciences, 1982
Research Award, Electrochemical Division, The Electrochemical Society, 1983
Carl Wagner Memorial Award, The Electrochemical Society, 1985
Professional Progress Award, American Institute of Chemical Engineers, 1985
Director, American Institute of Chemical Engineers, 1988-1991
G. W. Kidd Outstanding Alumnus Award, Lafayette College, 1988
E. V. Murphree Award, American Chemical Society, 1991
Technical Achievement Award, National Association of Corrosion Engineers, 1992
Lifetime National Associate, U.S. National Academies, 2002
Vittorio de Nora Award and Gold Medal, Electrochemical Society, 2004
Fellow, International Society of Electrochemistry, 2006
Invited Lecture Series, Waseda University, Tokyo, Japan, 2006
Ralph Peck Memorial Lecture, University of Illinois Chicago Institute of Technology, 2006
Distinguished Speaker Series, University of California, Riverside, 2006

Richard D. Braatz
Doctoral Thesis Prize, Hertz Foundation, 1994
DuPont Young Faculty Award, 1995
Teaching Excellence Award, University of Illinois School of Chemical Sciences, 1997
Advisors List for Advising Excellence, University of Illinois College of Engineering, 1999, 2002
Xerox Award for Faculty Research, University of Illinois College of Engineering, 1999
Donald P. Eckman Award, American Automatic Control Council, 2000
Council of Outstanding Early Career Engineers, Oregon State University, 2000
Ernest W. Thiele Lectureship, University of Notre Dame, 2001
Beckman Associate, University of Illinois Center for Advanced Study, 2002
University Scholar, University of Illinois, 2003
CAST Director's Award, American Institute of Chemical Engineers, 2003
Curtis W. McGraw Research Award, American Society for Engineering Education, 2004
Outstanding Paper Award, IEEE Transactions on Control Systems Technology, 2005
CAST Outstanding Young Researcher Award, American Institute of Chemical Engineers, 2005
Antonio Ruberti Young Researcher Prize, Institute of Electrical and Electronics Engineers, 2005
Lindsay Distinguished Lecturer, Texas A & M University, 2005-2006
Millennium Chair of Chemical and Biomolecular Engineering, University of Illinois, 2006
Excellence in Process Development Research Award, American Institute of Chemical Engineers, 2006
Fellow, Institute of Electrical and Electronics Engineers, 2007

**Thomas J. Hanratty, Emeritus**
Member, National Academy of Engineering
Member, National Academy of Sciences
Fellow, American Academy of Arts and Sciences
Fellow, American Physical Society
Honorary Doctorate, University of Toulouse
Honorary Doctorate, Villanova University
Allan P. Colburn Award, American Institute of Chemical Engineers, 1957
Curtis W. McGraw Award, American Society for Engineering Education, 1963
William H. Walker Award, American Institute of Chemical Engineers, 1964
Professional Progress Award, American Institute of Chemical Engineers, 1967
Senior Research Award, American Society for Engineering Education, 1979
Shell Distinguished Chair in Chemical Engineering, University of Illinois, 1981-1990
Distinguished Engineering Alumnus, Ohio State University, 1984
Ernest Thiele Award, Chicago Section, American Institute of Chemical Engineers, 1986
University Scholar, University of Illinois, 1987

J. W. Westwater Professorship, University of Illinois, 1989-1997
Lamme Medal, Ohio State University, 1997
International Prize for Research in Multiphase Flow, 1998

**Jonathan J. L. Higdon**
Presidential Young Investigator Award, National Science Foundation, 1984
Teaching Excellence Award, University of Illinois College of Liberal Arts and Sciences, 1988
Teaching Excellence Award, University of Illinois School of Chemical Sciences, 1984, 1986, 1990, 1994
Stanley Corrsin Lectureship in Fluid Mechanics, Johns Hopkins University, 1993

**Paul J. A. Kenis**
Akzo-Nobel Graduate Fellowship, 1993-1997
TALENT Postdoctoral Fellowship from NWO, Dutch Science Foundation, 1998
3M Young Faculty Award, 2001-2004
Collins Scholar, Academy for Excellence in Engineering Education, University of Illinois College of Engineering, 2001
Faculty Early Career Development Program (CAREER) Award, National Science Foundation, 2005-2010
Xerox Foundation Award for Faculty Research, University of Illinois College of Engineering, 2006
Excellence in Teaching Award, University of Illinois School of Chemical Sciences, 2006
Beckman Fellow, University of Illinois Center for Advanced Study, 2007-2008
Helen Corley Petit Scholar, University of Illinois College of Liberal Arts & Sciences, 2007-2008

**Hyun Joon Kong**
Fellowship Award, Hanyang University, 1988-1989
Fellowship Award, Samnam Foundation, 1990-1991
Honored Student, 1992
International Fellowship, Hanyang University, 1995-1997

**Mary L. Kraft**
Kirschstein Postdoctoral Fellowship, 2003-2007
Career Award at the Scientific Interface, Burroughs Wellcome Fund, 2007-2011

**Deborah E. Leckband**
Reid T. Milner Professor of Chemical Sciences
Fellow, American Institute of Medical and Biological Engineering (AIMBE)
Fellow, American Association for the Advancement of Science (AAAS)
National Science Foundation Research Initiation Award, 1993-1996
FIRST Award, National Institutes of Health, 1993-1998
Faculty Early Career Development Program (CAREER) Award, National Science Foundation, 1995-1999
Amoco Lectureship, Stanford University, 1998
Xerox Faculty Research Award, University of Illinois College of Engineering, 1998
Helen Petit Professorship, University of Illinois College of Liberal Arts and Sciences, 1999-2000
Fellow, University of Illinois Center for Advanced Study, 1999-2000
University Scholar, University of Illinois, 2001-2004
Plenary Speaker, American Chemical Society Colloids and Surface Science Symposium, 2001
Keynote Speaker, University of Virginia Bioengineering Symposium on Biomechanics of Adhesion, 2002
Provost's Distinguished Lecture Series, University of Texas, Austin, 2003
Distinguished Lecturer, Cell and Molecular Biology, Boston University School of Dental Medicine, Boston, 2003
Britton Chance Distinguished Lecturer in Engineering and Medicine, University of Pennsylvania, 2004
Fellow, American Institute of Medical and Biological Engineering (AIMBE), 2005-
Fellow, American Association for the Advancement of Science, 2006-

Richard L. Masel
Alumni Achievement Award, Liberal Arts College, 1996-1997
Postdoctoral Fellow, NATO, 1977
Exxon Faculty Fellowship in Solid-State Chemistry, American Chemical Society, 1982
Presidential Young Investigator Award, National Science Foundation, 1984
Innovation Discovery Award, 2005

Daniel W. Pack
Excellence in Teaching Award, School of Chemical Sciences, University of Illinois, 2000
Selection to Frontiers of Engineering Symposium, National Academy of Engineering, 2002
Faculty Early Career Development Program (CAREER) Award, National Science Foundation, 2002
Excellence in Teaching Award, School of Chemical Sciences, University of Illinois, 2003
3M Young Faculty Award, 2003-2006

Beckman Fellow, Center for Advanced Study, University of Illinois, Urbana-Champaign, 2004-2005
Multi-Year Faculty Achievement Award, College of Engineering, University of Illinois, Urbana-Champaign, 2007

Nathan D. Price
Bioengineering Department's Nominee for Campus Dissertation Prize, University of California, San Diego (UCSD), 2005-2006
Sam E. and Kathleen Henry Postdoctoral Fellowship, American Cancer Society, 2005-2007
Tomorrow's Principle Investigator Award, Genome Technology, 2007

Christopher V. Rao
Faculty Early Development Program (CAREER) Award, National Science Foundation, 2007
David Smith Jr. Paper Award, American Institute of Chemical Engineers, 2007

Nikolaos V. Sahinidis
DuPont Young Faculty Research Initiation Grant, University of Illinois, 1991
Faculty Early Career Development (CAREER) Award, National Science Foundation, 1995
Fellowship, National Science Foundation/Lucent Technologies Industrial Ecology, 1998
CAST Director's Award, American Institute of Chemical Engineers, 1999
INFORMS Computing Society Prize, Institute for Operations Research and the Management Sciences, 2004
Center for Advanced Study Associate, University of Illinois, 2005
University Scholar, University of Illinois, 2005
Beale-Orchard-Hays Prize Mathematical Programming Society, 2006

Edmund G. Seebauer
Dow Teaching Excellence Award, 1988
Presidential Young Investigator Award, National Science Foundation, 1988
DuPont Young Faculty Award, 1989
Fellow, Alfred P. Sloan Foundation, 1994-1996
Inventor Recognition Award, Semiconductor Research Corp., 1995
Teaching Excellence Award, University of Illinois School of Chemical Sciences, 1996
Fellowship for Study in a Second Discipline, University of Illinois, 2000
Fellow, American Vacuum Society, 2000
Distinguished Lecturer, Institute of Electrical and Electronic Engineers Electron Device Society, 2004-2006
Beckman Associate, Center for Advanced Study, University of Illinois, 2004
Excellence in Advising Award, College of Engineering, University of Illinois, 2005
James W. Westwater Professor, University of Illinois, 2006
Fellow, American Association for the Advancement of Science, 2007
Fellow, American Physical Society, 2007

**Michael S. Strano**

Sidney A. Savitt Award for Academic Excellence in Chemical Engineering, Polytechnic University, 1997
Garrett Reed Cantwell Graduate Scholarship, University of Delaware, 1998
Annual Research Award, Philadelphia Catalysis Society, 1999, 2001
Graduate Award, American Institute of Chemical Engineers Separations Division, 2001
Honorable Mention, Graduate Award, American Institute of Chemical Engineers Environmental Division, 2002
Young Investigator Award, Dupont, 2004
Top Young Innovator Award, MIT Technology Review, 2004
Faculty Early Career Development (CAREER) Award, National Science Foundation, 2005
Top 1% of Highly Cited Researchers, Essential Science Indicators/Web of Science, 2005
Young Investigator Award, Nanoscale Science and Engineering Forum, American Institute of Chemical Engineers, 2005
Coblentz Award for Molecular Spectroscopy, 2006
3M Nontenured Faculty Award, 2006
Beckman Young Investigator Award, 2006
Collaboration Success Award, Council of Chemical Research, 2006
Presidential Early Career Award for Scientists and Engineers (PECASE), 2006

**Huimin Zhao**

Dow Special Recognition Award, 1999-2000
Collins Scholar, University of Illinois College of Engineering, 2001
Faculty Early Development (CAREER) Program Award, National Science Foundation, 2004-2009

Excellence in Teaching Award, University of Illinois School of Chemical Sciences, 2004
Beckman Fellow, University of Illinois Center for Advanced Study, 2005-2006
Xerox Award for Faculty Research, University of Illinois College of Engineering, 2005
Dupont Young Professor Award, 2005
Helen Corley Petit Scholar, University of Illinois College of Liberal Arts and Sciences, 2006
University Scholar, University of Illinois, 2007
Investigator Award, Division of Biochemical Technology, American Chemical Society (ACS), 2008

**Charles F. Zukoski**

Presidential Young Investigator Award, National Science Foundation, 1987
Everitt Award for Teaching Excellence, University of Illinois College of Engineering, 1992
Fulbright Teaching/Scholar Fellowship to visit the University of Melbourne, 1992
Robert W. Vaughan Lectureship in Chemical Engineering, California Institute of Technology, 1993
Alumni Professor, University of Illinois Department of Chemical Engineering, 1994-1999
Thiele Lectureship in Chemical Engineering, Notre Dame University, 1994
University Scholar, University of Illinois, 1994-1997
Plenary Lecture: 13th Symposium on Industrial Crystallization, Toulouse, France, 1996
Moulton Medal, Institute of Chemical Engineers, 1997
Publication Award, Society of Rheology, 1997
Ralph K. Iler Award, American Chemical Society, 1997
Alcoa Plenary Lecture, Symposium on Particulate Fluids, Melbourne, Australia, 1998
William H. and Janet G. Lycan Chair, School of Chemical Sciences, University of Illinois, 2000-2001
Wilhelm Lectureship, Princeton University Department of Chemical Engineering, 2001
Engineering Council Award for Excellence in Advising, University of Illinois, 2002
Alpha Chi Sigma Award for Chemical Engineering Research, American Institute of Chemical Engineers, 2002
Member, National Academy of Engineering, 2007