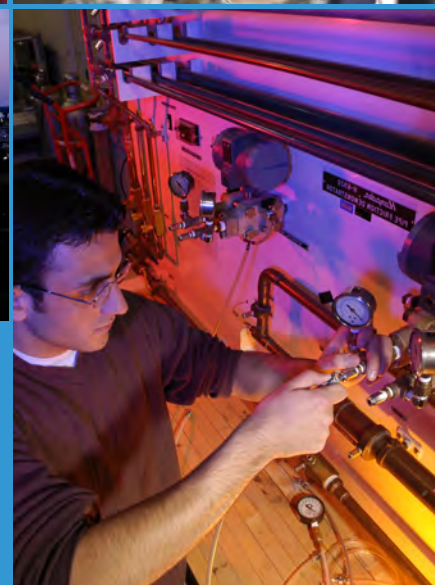
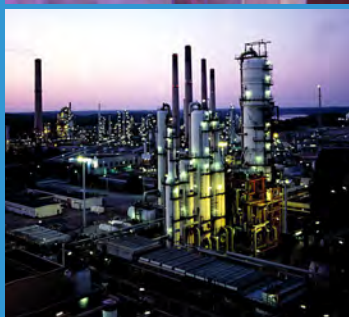
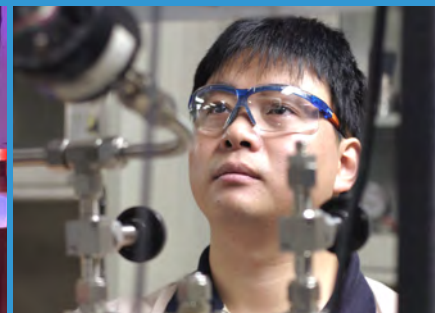


UNIVERSITY OF ILLINOIS AT CHICAGO

# Department of Chemical Engineering

Graduate Studies



## Message from the Department Head



Dear Prospective Graduate Student:

We are delighted that you are considering the UIC Department of Chemical Engineering to pursue your advanced studies. We offer outstanding, well-balanced, research-oriented programs leading to master's and doctoral degrees.

This is a very exciting time for the department, beginning with the advent of the Center for Innovation in the Chemical Industry. We have hired a new faculty member this year and plan to add several more over the next five years.

Chemical engineering at UIC is well known in disciplines such as fluid mechanics, catalysis, combustion, and molecular modeling. In addition to our continued emphasis on these core strengths, we have embarked upon exciting new research. In order to address the emerging research issues of national and international importance, we have structured the ongoing research efforts into three major interdisciplinary areas: Nanotechnology, Computing and Information Technology, and Infrastructure and Energy/Environmental Technologies.

As a graduate student in the chemical engineering department, you will work side-by-side with award-winning faculty who are leaders in their fields and well known nationally and internationally. The department consists of nine faculty members, five adjunct faculty, approximately 50 graduate students and 100 undergraduate students. Our faculty includes Fellows of professional societies, editors of various international journals, and winners of prestigious research awards such as the National Science Foundation CAREER Award.

PhD students conducting research under the supervision of their faculty advisors have also won many awards, such as university fellowships; dean and provost awards; the Abraham Lincoln fellowship; and FMC, GEM and IMGIP fellowships.

We are very proud of our state-of-the-art research laboratories, first-rate computational and experimental facilities and congenial atmosphere for graduate studies. Choosing to pursue graduate study and finding the right place to do so are highly important decisions. I encourage you to learn as much as you can about our programs. Visit the department, look over our faculty research profiles on our Web site, talk to our faculty, and meet with our students. I hope you will find that UIC's Department of Chemical Engineering offers the breadth and vision that you seek in a graduate program. I invite you to consider becoming a part of this talented and dynamic community.

*Sohail Murad*

Sohail Murad  
Professor and Head  
UIC Department of Chemical Engineering

## Graduate Program

The UIC Department of Chemical Engineering offers a Master of Science and a Doctor of Philosophy in Chemical Engineering. Typically, the MS degree requires two years of study while the PhD requires four to six years, depending on the candidate's background. Students entering with an MS degree in engineering typically require less time to complete their PhD, while students entering with a BS degree in a related field, such as chemistry, will require more time.

### Admissions

The department is highly oriented toward the PhD degree with a strong emphasis on research and scholarship. Presently, the department maintains a 2-to-1 ratio of PhD candidates to MS candidates. Applicants typically enter with either a BS or MS degree in chemical engineering. However, the department also accepts students with degrees from other engineering disciplines and related sciences such as chemistry, physics and biology.

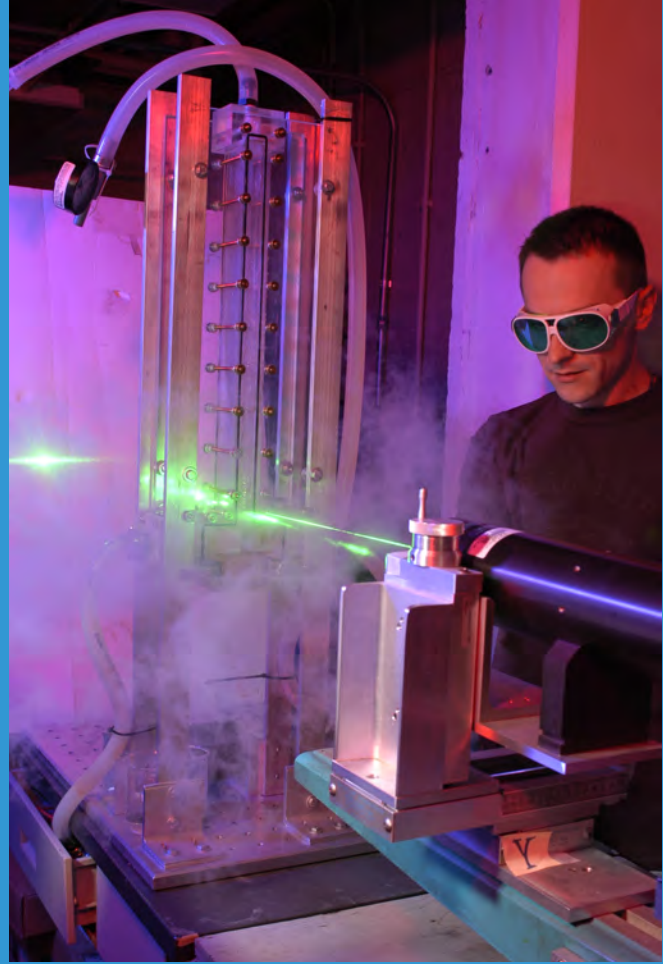
### Financial Aid

The department makes a concerted effort to support all PhD candidates who are making progress toward their degree. Incoming PhD candidates may be supported on teaching assistantships, fellowship awards or research assistantships. In subsequent years, PhD students are typically supported on research assistantships. Candidates for the MS degree may receive financial aid subject to the availability of funds; however, such aid is limited. MS candidates should plan to support themselves.

### Graduate Research

The PhD program in chemical engineering is focused on research which culminates in a thesis. Our PhD candidates are required to take 12 courses: five required core classes that form the foundation of the chemical engineering discipline, five elective courses that allow the student to explore research-related topics, and two mathematics courses to give the student a firm background in theoretical analysis. Students choose their courses and thesis topics in conjunction with their thesis advisors. The program allows the student and advisor to work together to tailor courses and research to current topics and specific interests. There is a strong emphasis on multidisciplinary research.

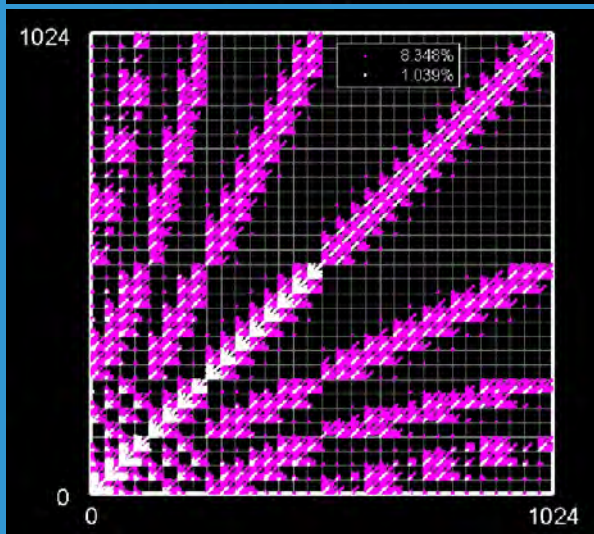
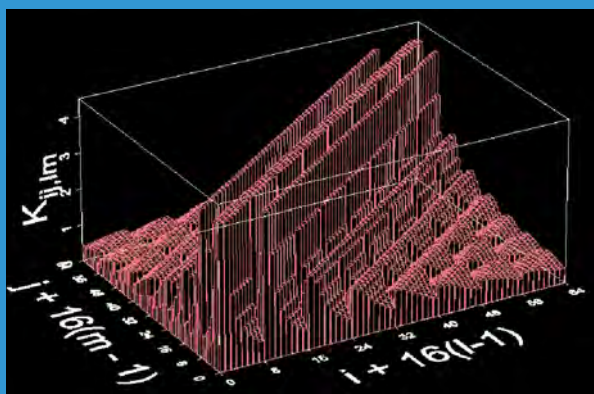
The MS program has two options: a thesis-based degree or a project-based degree. The thesis option requires the same five core courses as the PhD, plus one elective. This option emphasizes the research and style of the PhD, but in a more limited scope. Our course-work-oriented project option requires the five core courses plus three electives. In place of a thesis, the student writes and presents a project report.



# Areas of Emphasis

## Multiscale Computer Simulation of Complex Materials and Nanostructures

The UIC Department of Chemical Engineering is a focal point of computational and theoretical research in transport phenomena of systems with complex structures. The expertise of Professors Sohail Murad, Ludwig Nitsche, Raffi Turian and Lewis Wedgewood in molecular dynamics, particle simulation techniques and smoothed particle hydrodynamics, and stochastic simulations with both traditional and substructural continuum field theory, presents a unique interdisciplinary research vision to help unlock the technological potential of nanoscale, macromolecular, colloidal, microfluidic and interfacial processes. This is an arena where fundamental mechanistic understanding complements experimental techniques, and aids in design of nanotechnology, microfluidics and lab-on-a-chip systems.



### Integrated Computational Methodology

The computational core of our interdisciplinary research effort is a hierarchy of mesh-free, particle-based simulation techniques that interface with each other to form a continuous bridge between detailed molecular models and continuum theory. Particle methods deal naturally with intricate and changing multiphase and interfacial geometries, thus avoiding the geometric complexity and computational overhead of grid generation.

Another strength in the department is molecular dynamics (MD) simulations. MD provides a realistic picture of structure and transport on the Angstrom-nanometer scale, and represents a mechanistic final arbiter.

Particle simulation techniques interpose an “interaction kernel” between the discrete particulate structure and forces, and the resultant particle motions. This additional layer of information can be tuned smoothly from pure molecular to pure continuum, and vastly extends the scales in length and time to which pseudo-molecular modeling can be applied. Wavelet compression and other fast summation techniques are used to accelerate the calculation of particle interactions.

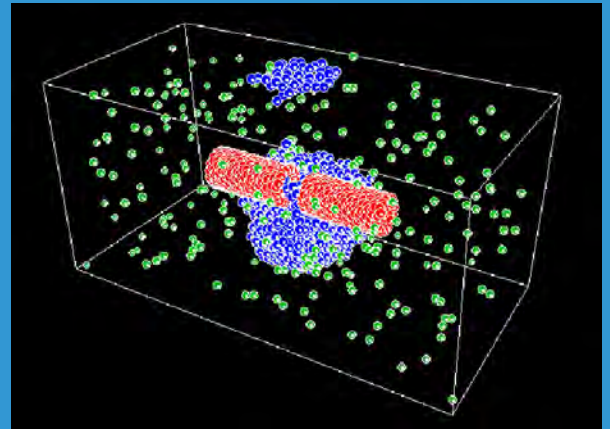
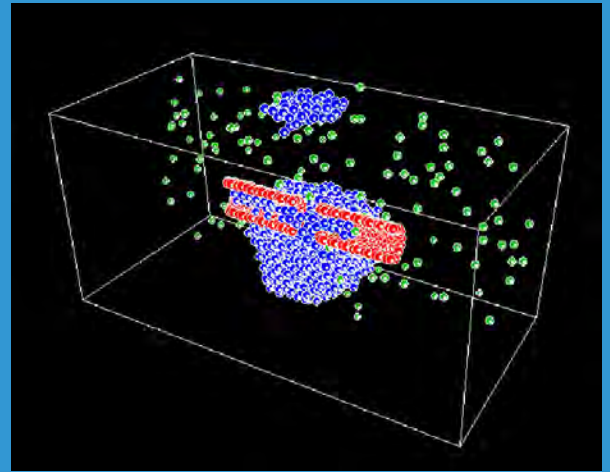
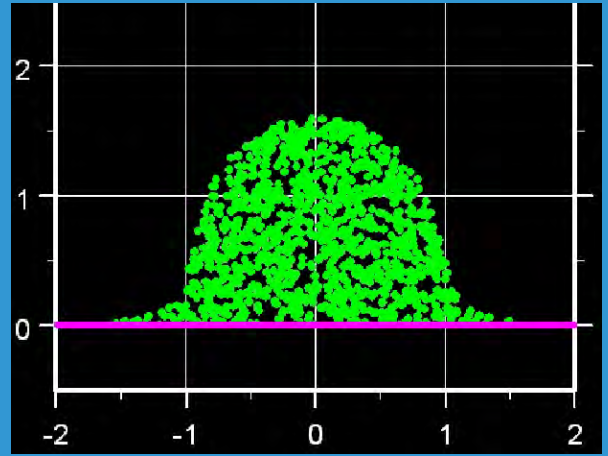
Stochastic simulations make a complementary but different separation of effects, in treating dissolved/suspended molecules/particles as discrete entities while modeling the solvent as a continuum bath. Molecular fluctuations due to the bath are modeled with stylized random forces (possessing well-defined statistics), which greatly speed up the computations compared with full MD. Stochastic simulations are not confined to mass transport, and can be applied equally to heat transfer as well as abstract quantities and generalized internal degrees of freedom of polymer chains for rheological modeling.

Reaching down in scale from continuum theory, and based upon the insights obtained from particle simulations, substructural models provide concise mathematical descriptions of the extra information from the microscopic or molecular scale that affects observable material response functions but is otherwise inaccessible to the continuum view. Asymptotic theory and approximation techniques are merged with the numerical simulations and exploited where possible to enhance computational efficiency.

## Complex Fluids and Structures

Our scale-transcendent computer simulation capability unlocks detailed mechanistic analysis and provides engineering design targets for nanoscale, microfluidic and colloidal systems. Previous successes and applications under development that benefit from combining molecular and substructural continuum theory include:

- Desalination of sea water with nanoporous reverse-osmosis membranes
- Infiltration of carbon nanotubes with water, and modulating effects of electric fields
- Movement, coalescence, mixing and reaction of microdroplet reactors in microchannel lab-on-a-chip systems, and control through electro-wettability effects
- Colloidal flow, interfacial transport and adhesion processes in mineral flotation processes



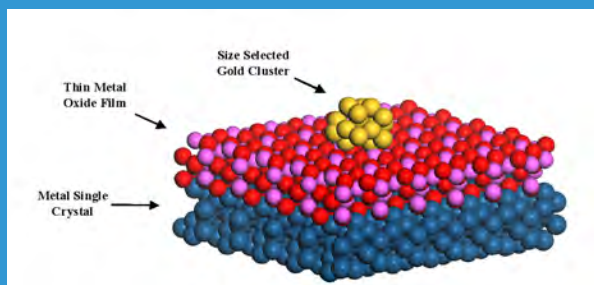
# Areas of Emphasis



## Catalysis and Surface Science

### Cluster Catalysis

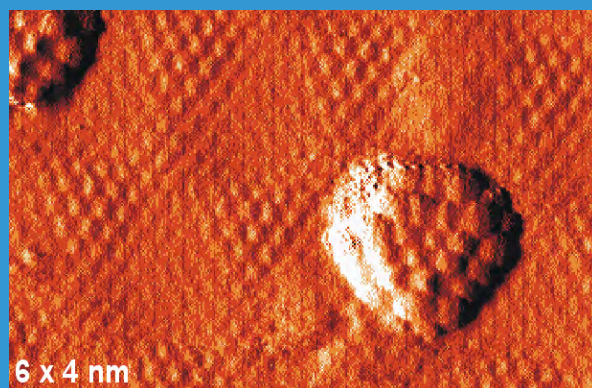
Professor Randall Meyer's research involves the construction of well-defined model systems both experimentally and computationally in concert, which allows in-depth investigation of structure-reactivity relationships at the molecular and atomic level. Model catalysts, consisting of metal particles supported on thin film or single crystal metal oxide surfaces, have been utilized successfully for more than a decade in an effort to understand particle size and support effects in catalysis. His work, with the aid of collaborators from the Cluster Studies Group at Argonne National Laboratory, employs model catalysts with mass-selected clusters in order to examine size and composition effects on an atom-by-atom basis. Supporting the experiments at Argonne, his group employs *ab initio* (from first principles) quantum chemical calculations to gain additional insight into experimental results. *Ab initio* methods have proven to be a most useful tool in quantum chemistry. These methods allow for the calculation of accurate electronic structures for solid materials and their interactions with adsorbates on an atomic scale. Ultimately, we can obtain an understanding of the rate-limiting step for a given reaction, and design novel catalysts.



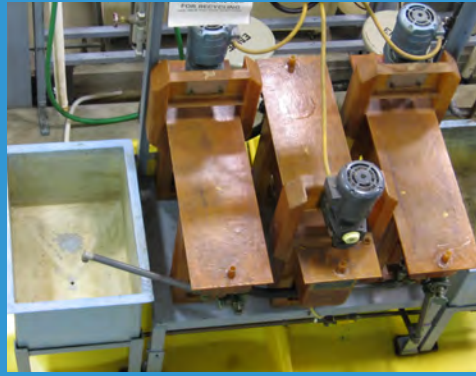
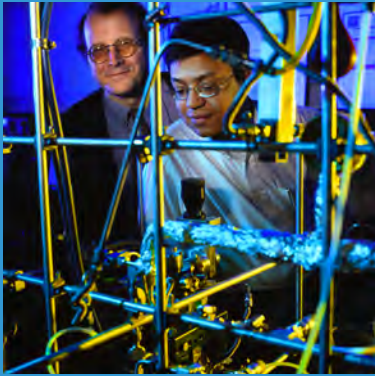
Model catalyst constructed from deposition of size-selected clusters on a thin metal oxide film above a metal single crystal substrate.

### Microelectronic Materials and Processing

Professor Christos Takoudis' major thrust is in relationships among processing, properties and structure, as well as the development of new materials and processes. Objectives include novel substrate surface cleaning techniques; kinetics and surface chemistry of reaction processes on silicon substrate surfaces; controlled production of thin heterostructure layers; and design of new material systems for fabrication of group IV-based optical, electronic and micro-electro-mechanical systems. Specific systems of interest include silicon selective epitaxial growth, silicon-germanium growth, ultra thin silicon oxynitride films and *in situ* probing of surface chemical phenomena during the thin film growth of microelectronic materials.

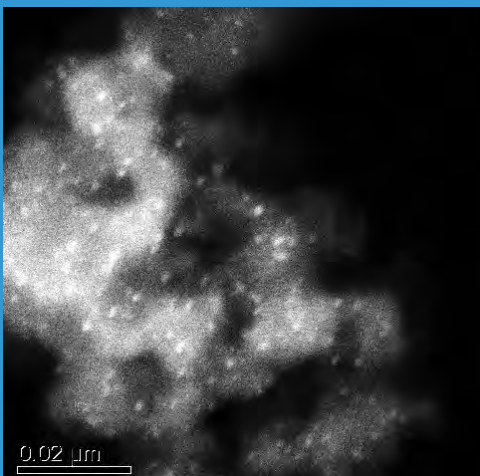


STM image of 2 nm monolayer gold cluster on a thin iron oxide film. Image from the Chemical Physics Department at the Fritz Haber Institute in Berlin, Germany.



## Catalyst Preparation

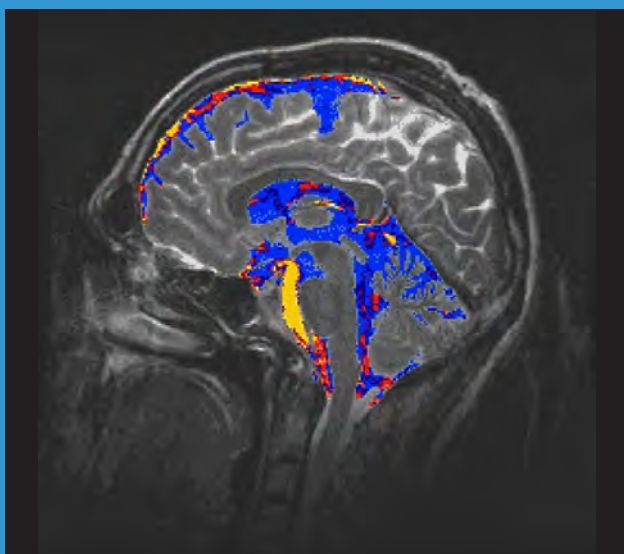
Professor John Regalbuto's lab has undertaken the fundamental study of catalyst preparation. His approach centers on a simple electrostatic model of metal adsorption. This understanding has led to better ways to make Pt/carbon fuel cell electrocatalysts (below). The tiny bright specks are Pt particles about one nanometer in diameter. The smallest metal particles yield the highest possible catalytic activity by exposing the greatest amount of metal. After catalysts are prepared, they are characterized by state-of-the-art instrumentation like electron microscopy and x-ray photoelectron spectroscopy at UIC, and x-ray absorption spectroscopy at the Advanced Photon Source at Argonne National Laboratory.



# Areas of Emphasis

## Process Modeling and Design

The department is applying the tools of chemical engineering to model and design processes from length scales of nanometers to large plant operations. Some of the most exciting and relevant research develops new processes that are faster, better, cheaper, sustainable and environmentally benign. Applications range from biomedical to industrial. Graduate students are directly involved in this research effort.



### Modeling of Complex Fluids in Complex Flows

A research project led by Professor Lewis Wedgewood addresses the flow of blood through arteries to understand the process that leads to atherosclerosis. Here blood is modeled as a complex suspension of cells, proteins and other constituents. Flow bifurcations where stenoses (i.e., constrictions) typically form are studied to determine the mechanism behind the life-threatening disease.

Research led by Professor Andreas Linninger models the pulsating flow of the cerebrospinal fluid in the brain in order to improve treatment of hydrocephalus. The goal of the research is to understand the transport mechanism of therapeutic drugs and various drug infusion policies for the treatment of neurological diseases including brain tumors, epilepsy and Parkinson's disease. Specific attention is given to emerging inversion problem techniques capable of adjusting the design variables of the therapy to the desired targets specified by the physician.

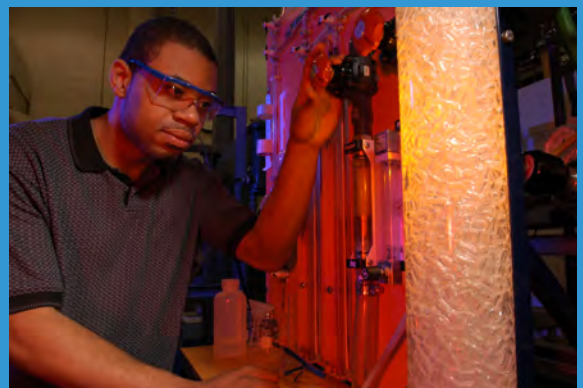
The dynamics of droplets in confined geometries and microchannels is being studied by Professor Ludwig Nitsche, in order to develop predictive computational design techniques for lab-on-a-chip micro total analysis systems. Microscopic droplets function as mixers and reaction vessels in biochemical assays and analytical and combinatorial chemistry. These inherently nonlinear, free-surface problems involve complex interactions between viscous and interfacial forces and external fields, and involve breakup, coalescence and reaction phenomena.



The study of both dilute and concentrated polymeric systems is of continuing interest to both Professors Nitsche and Wedgewood. Systems of polymer melts are being modeled as temporary junction networks in order to capture the mechanical properties of these fluids.

Another system of interest is ferrofluids where the rotation of nanoscale metallic particles can be manipulated by external electromagnetic fields. Ferrofluids present an exciting challenge to model and understand. Ferrofluids are already found in exciting applications such as drug delivery, high-speed printers and microheat transfer.

Professors Nitsche and Wedgewood have also collaborated on melding computer simulations with asymptotic theory to model dilute polymer solutions in elongational flows. The result is a set of accurate macroscopic constitutive equations for the notably difficult problem of transient stresses and hysteresis loops in stress-birefringence.



## UIC Department of Chemical Engineering Industrial Advisory Board

In order to stay abreast of chemical engineering industry needs, and to continue corporate relationships that can provide students internships or jobs, we have assembled an impressive team of experts on our advisory board.

**Dr. Normal Li**

President and CEO  
NL Chemical Technology, Inc.

**Dr. Samuel Wong, PE**

Senior Process Engineer  
Chevron Phillips Chemical Company

**Dr. Anil Oroskar**

Chief Technology Officer  
Orochem Technologies Inc.

**Dr. Diane J. Graziano**

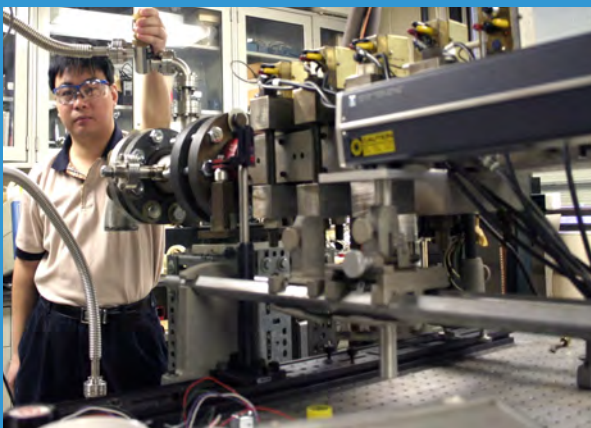
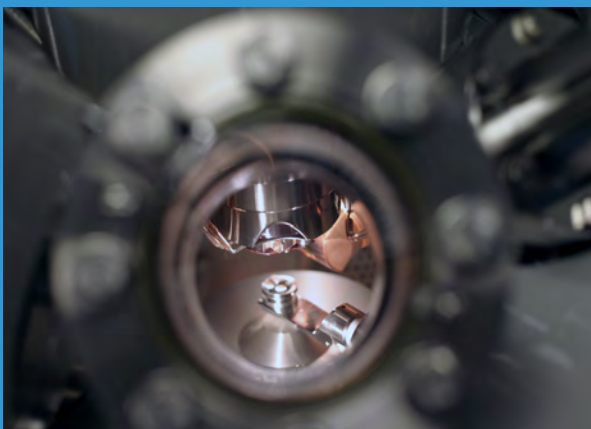
Deputy Division Director  
Argonne National Laboratory

**Dr. S. S. Kumaran**

Sr. Research Engineer, Global Operations  
Cabot Corporation

**Dr. John F. Hardin**

President  
LA-CO Industries



## Center for Innovation in the Chemical Industry

In order to meet the challenges of the 21st century, there is an urgent need to renew the technologies of the chemical industry and start another century of innovation. With innovation and a renewal of primary chemical processes in the chemical and energy sector as the goal, a Center for Innovation in Chemical Industry has been established at UIC.

The center is led by Professor Anil Oroskar. Projects are developed by the faculty and are voted upon by a steering committee of industry representatives that the center serves. Center participants include undergraduate students, graduate students, post-doctoral Fellows and faculty. The center makes special efforts to ensure diversity among all participants and closely works with university offices dedicated to such diversity.

The basic philosophy of the center is to gather a group of highly talented and skilled research and development scientists/engineers to fuel innovation and help power performance and growth in the refinery and chemical industries. The creative energies of the center focus on increasing efficiencies, solving business challenges by lowering costs and producing products with greater value. This is accomplished via process integration, process intensification and miniaturization, and distributed production.

In the current competitive business environment, it is no longer possible for every business to carry out all the fundamental and applied research needed to develop such innovative technologies. Partnerships via the center fill a crucial need to approach technology innovation more efficiently and economically, thus avoiding costly duplication of efforts. This partnership enables the chemical and oil industries to share technical risks, costs and talents with others that have complementary capabilities.

The chemical industry has had a significant innovation cycle during the past 100 years, but this industry is now showing signs of technological maturity with the rate of innovation slowing down considerably during the past 25 years. Unfortunately this technological maturity is on the heels of significant growth of demand for energy as well as a shortage of fossil fuels around the world.

# Faculty



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Phone: (312) 996-2581; E-mail: [linninge@uic.edu](mailto:linninge@uic.edu)  
Product and process development and design, computer-aided modeling and simulation, pollution prevention



Sohail Murad, Professor and Head  
PhD, Cornell University, 1979  
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Statistical thermodynamics and computer simulation studies of dense fluids and mixtures; engineering correlations for thermodynamic and transport properties



G. Ali Mansoori, Professor  
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Applied statistical mechanics and thermodynamics, supernatural fluid extraction/retrograde condensation, asphaltene characterization and deposition



Randall Meyer, Assistant Professor  
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Density functional theory calculations of reaction mechanisms; properties of size selected clusters



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Particulate and macromolecular transport in porous materials, multiphase flow, nonlinear drift effects in Brownian diffusion, antisedimentation dialysis of macrolutes, applied mathematics, numerical fluid mechanics, centrifugal fan aerodynamics



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Heterogeneous catalysis; fundamental theory of catalyst preparation; characterization of solid catalysts; in-situ characterization of catalyst preparation; heterogeneous reaction kinetics



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Phone: (312) 355-0859; E-mail: [takoudis@uic.edu](mailto:takoudis@uic.edu)  
Microelectronic materials and processing, micro-fabrication techniques, chemical sensors, micro-electro-mechanical systems (MEMS), heteroepitaxy in group IV materials; in situ surface spectroscopies at interfaces, heterogeneous catalysis, novel approaches to reaction kinetics, reaction engineering



Raffi M. Turian, Professor  
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Characterization, stability, rheology and flow behavior of complex fluids; microbial desulfurization of coal; perturbation and approximation methods applied to transport processes



Lewis E. Wedgewood, Associate Professor and Director of Graduate Studies  
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Non-Newtonian fluid mechanics; polymer kinetic theory, molecular-level simulation of complex liquids including ferrofluids and biological fluids, continuums mechanics, laser-Doppler velocimetry

## Adjunct and Emeritus Faculty

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Bryce A. Williams, Adjunct Professor  
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## Living in Chicago

The University of Illinois at Chicago is the largest university in the Chicago area, with 25,000 students and 15 colleges. It is among the top 50 universities in federal research funding, totaling more than \$290 million annually. The College of Engineering is proud of its academic excellence, the 1550 undergraduate and 850 graduate students, and its 115 faculty. Two faculty are members of the National Academy of Engineering, and others have earned numerous prestigious awards.

UIC is in a great location within walking distance of the Chicago Loop business district. Chicago is home to many international companies including Abbott, Baxter Healthcare, British Petroleum, General Electric and Universal Oil Products.



Students and faculty can enjoy 29 miles of lakefront that stretches alongside downtown, and take full advantage of the city's great nightlife, restaurants, shopping, museums and sports. The Chicago and UIC experience includes many diverse neighborhoods, which are represented by nationalities from all over the world.

[www.che.uic.edu](http://www.che.uic.edu)

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**UIC** COLLEGE OF  
UNIVERSITY OF ILLINOIS  
AT CHICAGO ENGINEERING