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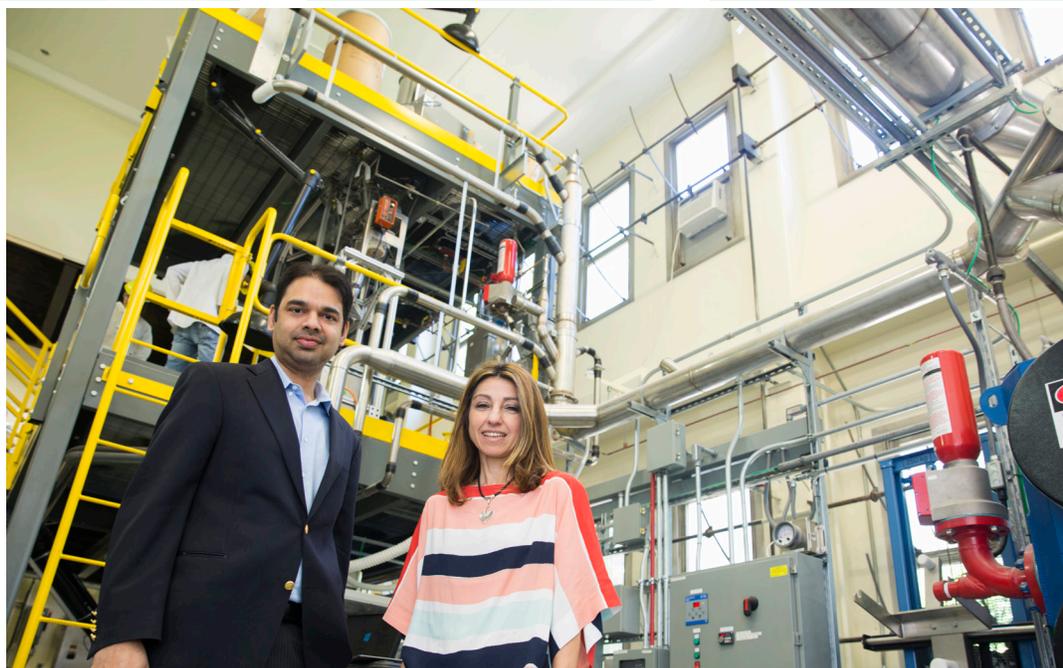
Professor Chundawat's Research Team Characterizes Biofuel Enzymes

Chemical & Biochemical Engineering at Rutgers

Chemical engineering sees a growing role in today's society advancing innovation across virtually every industry. The Department of Chemical and Biochemical Engineering at Rutgers has spearheaded critical research in areas that include biotechnology and bioengineering, materials, pharmaceutical science and engineering, and process systems and reaction engineering, among other new fields of study.

cbe.rutgers.edu

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CBE Playing Key Role in Transforming Pharmaceutical Manufacturing

In the decade since receiving a grant from the National Science Foundation (NSF) that would establish the Engineering Research Center for Structured Organic Particulate Systems (C-SOPS), the Department of Chemical and Biochemical Engineering has advanced the ambitious goal of transforming pharmaceutical manufacturing in much the same way engineers modernized the petroleum refining business more than three decades ago.

Beginning in the early 1980s, crude oil prices began dropping dramatically, and they would continue dropping for the next two decades. So manufacturers turned to engineers to develop a number of advances to optimize their processes and improve profitability while guaranteeing quality. Today, if you walk into the control room of a typical refinery, you will see sophisticated control systems that are constantly monitoring and adjusting the refining process.

These days, drug makers are under financial pressures, as more and more medicines lose patent protection and companies must compete with cheaper generic versions. So the industry is turning to Rutgers and its experts who are working to modernize manufacturing practices that have changed little in decades, and figure out ways to make medicines more quickly and efficiently – sometimes before the actual manufacturing has ever begun.

The Rutgers team already has taken an important first step with the implementation process called continuous manufacturing, led by **Fernando J. Muzzio**, distinguished professor, Department of Chemical and Biochemical Engineering, one of the lead investigators on the original NSF grant.

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Graduate Research Symposium

The Department of Chemical and Biochemical Engineering held the second annual Graduate Research Symposium in November to help doctoral and master's degree students network with potential employers, as well as present their research to their peers and corporate representatives.

Dr. Gregory Russotti, vice president of technical operations at Celgene Cellular Therapeutics and Rutgers CBE alumnus (pictured below), gave the keynote address and students interacted with employees from Merck, Janssen Pharmaceuticals, PepsiCo R&D, Bristol-Myers Squibb, and DuPont. Part of the event was designed to help the graduate students consider collaborations with one another to further aid their research. ■



Message from the chair

I am very excited to share with you the most recent news from the Department of Chemical and Biochemical Engineering.

Our department continues to grow in size and stature. We currently have 255 master's students, including 46 pursuing a master's of engineering and 130 doctoral students. This significant growth in our graduate program is thanks to the accomplishment of our faculty, particularly graduate director, Prof. Charles Roth, who has worked to recruit new students and support those who are here. In addition, we currently have 342 undergraduate students (sophomores through seniors) in the program, some of whom are highlighted in this newsletter for their achievements.

Our students were active this year in a number of events, including traveling to the annual AIChE meeting in Salt Lake City. Our graduate students once again took the lead in organizing a successful symposium showcasing their work to local industrial participants.

In the area of pharmaceutical advanced manufacturing, we are leading the way, receiving funding from NSF and FDA to accelerate the introduction of advanced modeling approaches in modernizing pharmaceutical manufacturing. Our partner Janssen recently received approval from the FDA to process tablets on a continuous manufacturing line at their plant in Puerto Rico. In keeping with that good news, we will be hiring a faculty member in the area of biopharmaceuticals to expand our activities and increase our presence in this area.

I know you will join me in celebrating our many successes!

Marianthi Ierapetritou, Ph.D.

Chair, Department of Chemical and Biochemical Engineering

faculty awards & news

AICE Fellow Recognition

Marianthi Ierapetritou, professor and CBE department chair, was elected a fellow of the American Institute of Chemical Engineers, recognizing her work and contributions to the field. She was awarded the Society of Powder Technology, Japan's Particulate Preparations and Design (PPD) award for her excellent work in continuous pharmaceutical processing.

Prabhas Moghe, CBE and BME distinguished professor, recently published a pioneering study on nanotherapeutics in Proceedings of the National Academy of Sciences, entitled, "Sugar-based Amphiphilic Nanoparticles Arrest Atherosclerosis In Vivo." The nanoparticles are targeted to block the transformation of macrophages into foamy cells, which set off inflammation processes early in the development of atherosclerotic plaques. Nanoparticle treatment successfully reduced arterial wall thickening and plaque formation in mice.

Prof. Moghe was also awarded a two-year Exploratory/Development Grant for \$424,000 along with co-PI Professor Zhiping Pang (Child Health Institute of NJ, RBHS) by the National Institute of Neurological Disorders and Stroke (NINDS) at the NIH for a project entitled "Nanofibrous Scaffolds for Transplantation of Human Dopaminergic Neurons." The ultimate goals are to develop better cell therapy models to study and treat neurodegenerative diseases like Parkinson's Disease.

Stavroula Sofou, CBE and BME associate professor, and her team were awarded a collaborative research \$569,000 NSF grant for the study of unique binding geometries. The research involves collective measurements as well as single molecule optical tracking techniques to develop and subsequently computationally test mechanistic hypotheses for the kinetics of binding between unique nanoparticle geometries and single receptors or assemblies of receptors,

leading to the design of high impact nanoparticles for theranostic applications.

Nina Shapley, CBE associate professor, has received NSF funding to explore sustainable dyes in collaboration with Jane Palmer of Noon Design Studio. The grant provides \$225,000 to develop a novel, robust, low pollution, and low-water-use natural dye process as an alternative to conventional synthetic textile dyes.

Shishir Chundawat, CBE assistant professor, was part of a team that has characterized critical biofuel enzymes using single-molecule techniques. A collaborative paper with the Lang Lab at Vanderbilt University outlining the single-molecule characterization of processive cellulolytic enzyme action on the surface of crystalline cellulose was published in Nature Communications. This study has revealed the individual biocatalytic steps

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The traditional method for manufacturing tablets involves combining huge batches of chemical compounds in gigantic mixers. Rutgers researchers, with additional funding from the Food and Drug Administration (FDA), have helped to develop a process that involves feeding the raw materials into a continuously running process, which can help companies cut costs and introduce new products more quickly. In a significant milestone, the FDA recently approved a new continuous manufacturing process at a plant in Puerto Rico operated by Janssen Supply Chain, a unit of Johnson & Johnson, culminating years of work with Rutgers and C-SOPS.

Now, as a next step, the researchers at Rutgers are turning their sights on the newest, most sophisticated manufacturing systems in the pharmaceutical industry – those used to produce “biologics.” This far more complex process uses cutting-edge tools of biotechnology and living organisms to produce large protein molecules that are made into injectable solutions, including some of the most widely used treatments for rheumatoid arthritis, multiple sclerosis, and a variety of cancers.

Marianthi Ierapetritou, professor and chair of the Department of Chemical and Biochemical Engineering, is a pioneer in the area of modeling and optimizing pharmaceutical manufacturing processes.



“We have come a long way, and the pharmaceutical industry, once lagging behind others, is changing rapidly,” said Ierapetritou, a major contributor to C-SOPS. “But this next step in biologics will take another five years.”

Her work in this field combines both experimental and computational components. The basic idea is that the manufacturing process can be reduced to a series of operations, and



each one can be described by mathematical equations. Once you develop these equations, you can model the process and predict how you can improve upon it by using a process called **Predictive Flowsheet Modeling**.

Ierapetritou was involved with the continuous manufacturing project from the beginning, developing models for each of the steps in the process, precisely describing the operation of equipment like feeders, hoppers, mixers, tablet presses and coaters that combine the active pharmaceutical ingredient with other compounds to produce the actual tablet.

Once these processes are modeled individually, you need to put them together to simulate the actual functioning of the manufacturing line. Then you can test the process and different variations to determine how best to optimize systems to reduce waste, maintain quality and meet stringent safety requirements.

Still, you need more than a theory and models to make it happen. You also need sensors and control systems to monitor and adjust the process as the products are being made.

That's where colleague assistant professor **Rohit Ramachandran** comes in.

He and his team are responsible for taking this kind of theoretical work and designing sensors and automated systems that can monitor and



Researchers at Rutgers are turning their sights on the newest, most sophisticated manufacturing systems in the pharmaceutical industry – those used to produce “biologics.”



control what is happening during the manufacturing process and allow operators to make rapid adjustments. Just as the predictive models analyze the behavior, he must find ways to measure and modify specific parameters, such as particle size, uniformity of the blend, moisture content, tablet thickness and hardness and the feed rate.

In addition, he develops systems to handle the massive amount of data that you need to monitor these complex processes. This means developing a cloud-based system that can be used to transmit data from the manufacturing plant to managers anywhere in the world who can take immediate action.

“Without these strategies, you won't know when you are getting bad product and, more important, you are not correcting it,” Ramachandran said.

Compounding the difficulty of this engineering work is that you must operate under the watchful eye of the FDA, which has developed its own protocol, **Process Analytical Technology**, to describe this shift from a static batch process to a more dynamic approach. The oversight by the FDA means significantly more scrutiny than for conventional manufacturing, given the direct impact on human health.

“Rutgers has been a center for this research for many years and is one of the leading institutions in this area,” Ierapetritou said. The FDA has funded her work with a \$4 million research grant, the largest of its kind. (That is in addition to an earlier \$2 million grant from the National Science Foundation.)

“There is a long tradition and history in the department of working with the pharmaceutical companies,” she added. “It's important for the state of New Jersey to establish a center of expertise like ours.” ■

involved in the action of cellulase enzymes on polysaccharide substrates for the very first time.

Meenakshi Dutt, CBE assistant professor, published several exciting results in the *Journal of Computational Chemistry*, *Journal of Physical Chemistry B*, and *AIMS Materials Science*. She also co-organized a symposium at the Materials Research Society Fall 2015 meeting entitled, "Modeling and Theory-Driven Design of Soft Materials," which was supported by NSF, AFOSR, and ARO.

Alex Neimark, CBE professor, was awarded a \$300,000 NSF GOALI (Grant Opportunities for Academic Liaison with Industry) for a research collaboration between Rutgers University and DuPont Corporation to support developing theoretical foundations for separation of functionalized nanoparticles using a new technique of interaction nanoparticle chromatography.

EPA's 2015 Scientific and Technological Achievement Award
Prof. Yannis Androulakis, **Meric Ovacik** (awarded Ph.D. 2010, now a senior scientist at Merck) and **Prof. Marianthi Ierapetritou**, along with EPA

collaborators, received the EPA's 2015 Scientific and Technological Achievement Highest Level Award, recognizing their work on toxicogenomic data in risk assessment.

New Book Published by Ierapetritou and Ramachandran

Professors Marianthi Ierapetritou and **Rohit Ramachandran** are the editors of *Process Simulation and Data Modeling in Solid Oral Drug Development and Manufacture*, a new book summarizing the recent developments in solid oral drug manufacturing.

Professor Alexander Neimark Honored by AIChE and Rutgers



Distinguished Professor Alexander V. Neimark was honored at a special Honorary Plenary Session on Adsorption and Ion Exchange at the 2015 annual meeting of the American Institute of Chemical Engineers, held in Salt Lake City in November 2015. Recognized for his seminal contributions in modeling and characterization of nanophases and nanostructured materials by the AIChE Separations Division, Neimark is an internationally renowned expert in adsorption science and engineering.

The honorary session featured lectures from some of Neimark's colleagues, including North Carolina State University's Keith Gubbins, Quantachrome Instruments' director

Matthias Thommes, Karl Johnson from the University of Pittsburgh, Peter Monson of the University of Massachusetts – Amherst, Shinshu University's Katsumi Kaneko, and Peter Ravikovitch from Exxon Mobil. His research interests include thermodynamics, statistical mechanics, and molecular simulation of nanoporous and self-assembled materials.

Neimark was also selected to receive the Rutgers Board of Trustees Award for Excellence in Research for the academic year 2015-2016. The BOT awards honor faculty members who have made distinguished research contributions to their discipline and/or society at large. ■

Meet Chemical and Biochemical Engineering Professor George Tsilomelekis

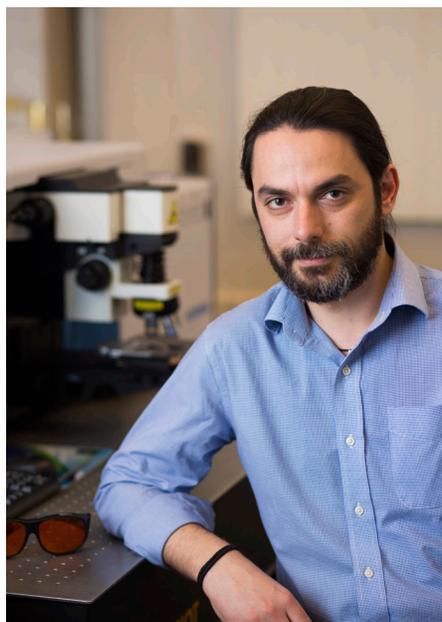
U.C. Davis Professor Presents Lecture

The Department of Chemical and Biochemical Engineering was delighted to welcome **Bruce C. Gates** to present the 2016 Distinguished Lecture in Chemical and Biochemical Engineering this spring. Gates is a distinguished professor of chemical engineering and materials science at the University of California, Davis. His research focus is catalysis, with an emphasis on molecular metal complex and metal cluster catalysts anchored to solid surfaces and on catalytic conversion of biomass-derived compounds.

His lecture, *Molecular Metal Catalysts on Supports: Organometallic Chemistry Meets Surface Science*, was presented on April 13, 2016 to an audience that included students, faculty, and alumni. Gates holds a bachelor's degree in chemical engineering from UC Berkeley, a doctoral degree from the University of Washington, and was the recipient of a Fulbright grant which included postdoctoral research at the Ludwig Maximilians University of Munich. Previously he was a research engineer at Chevron Research Company. ■



Dr. Gates joins Dr. Ierapetritou and other CBE faculty for dinner, following the lecture.



George Tsilomelekis, assistant professor of chemical and biochemical engineering, joined the School of Engineering in 2015 with extensive experience studying catalytic materials. Previously he was a postdoctoral research associate at the University of Delaware, studying solvent effects in biomass processing.

Tsilomelekis is pictured above with a state-of-the-art Raman spectrometer used in his research.

What classes do you teach?

I teach Chemical Engineering Kinetics which is an undergraduate core course in chemical engineering. This is an important course that utilizes knowledge from almost all the core courses in chemical engineering such as thermodynamics, transport phenomena and analysis, etc. I really enjoy teaching this course.

How do you bring that enthusiasm to your students?

I always try to incorporate examples from my research in the lectures that are well-connected to the "real-world." During these examples, students like to contribute to discussions and this dynamic approach allows them to take an active role in their own education.

What is your research focus?

Our research focuses on the establishment of structure-reactivity relationships in an effort to understand complex catalytic reactions in the

broader field of converting renewable and alternative energy sources (biomass and shale gas) to fuels and chemicals. Our approach is centered around the intersection of chemical engineering, chemistry, and material science in which we bring state-of-the-art operando spectroscopy as the enabling tool to answer key research questions.

Can you explain this technology?

Operando spectroscopy does not refer to a specific spectroscopic technique or instrumentation. Actually, it is a fairly new field of research in an effort to provide structure-performance relationships in catalysis in which we combine spectroscopy during catalytic reaction with simultaneous activity measurements at the same reactor. The main challenge in this field is to design and actually build an optical cell, in other words an "optical reactor" that allows the generation of catalytic performance data similar to those achieved with conventional catalytic reactors.

Why is this important and what are the implications of your research?

Predicting the behavior of catalytic materials has remained a long standing goal of the scientific community and has been enabled in recent years by advances in both experimental and theoretical frontiers. These are difficult problems which require us to think at a molecular level. This understanding improves our ability to discover better catalytic systems and provides an excellent opportunity for fundamental science with long-term impact on developing improved processes.

What do you like to do in your spare time?

It's been said that, "Music is enough for a lifetime, but a lifetime is not enough for music." To me, music is more than just something to do in your spare time. It was always my gateway to start thinking "out of the box." Music has been one of the most important and influential things in my life.

Do you play any instruments?

I do play a few instruments, but for the last 10-15 years I prefer to play the guitar. I think I'm among those people that believe in two kinds of music, "the good music and the other kind."

Do you have a favorite musician?

If I had to pick one favorite singer (among a huge pool of candidates) I'd pick Paul Rodgers. ■

CBE Students Distinguish Themselves Nationally



Six students created posters for the 2015 AIChE Undergraduate Poster Session detailing their research, with two being awarded for their efforts. Senior **Franklin Bettencourt**, also minoring in biochemistry, is analyzing different models of particulate systems under a grant by the National Science Foundation with his advisor, Prof. Rohit Ramachandran. He is also working with doctoral student **Anik Chaturvedi**. Bettencourt won second place for his poster on “Hybrid Parallelization of Population Balance Models for Massively Accelerated Modeling of Particulate Processes.”

Ajay Kashi created a poster explaining his work on analyzing how a particle’s size affects its electrochemical activity. The CBE junior won first place for his research conducted with the Rutgers Energy Institute under Dr. Anders Laursen. Kashi works in Dr. Charles Dismukes’ lab, where he developed his poster titled “Scalable Synthesis of Nanoscale Ni₅P₄ as a Noel HER Catalyst: Investigating the Correlation Between Particle Size and Electrochemical Activity.”

Katelyn Dagnall, **Sarah Libring**, **Nour Srouji**, and **Jacob Massa** also attended the AIChE Poster Competition, presenting work that analyzed how organic substances interact with titanium dioxide, viruses, light-interactions with polystyrene, and methanol formation.

CBE graduate students have also been productive over the past year – **Xiang Yu** and **Xiaolei Chu** earned a “best poster award” at the Materials Research Society fall 2015 meeting. Yu is working to earn his Ph.D. while Chu recently graduated with a master’s degree.

Ashu Tamraker, another Ph.D student, earned a travel award to present his research on powder mixing technology at the European Symposium on Computer-Aided Process Engineering.

Fikret Aydin, **Leebyn Chong**, and **Agnes Yeboah** also received travel awards from the Graduate School of New Brunswick to help them attend a conference.

Congratulations Class of 2016!

This year’s graduating class included 89 undergraduates, 53 master’s degree recipients, and 14 doctoral degree recipients. Five undergraduates were J.J. Slade Scholars and least nine graduates have been admitted to Ph.D. programs, including:

- **Katelyn Dagnall** (University of Virginia)
- **Charles Foster** (Penn State University)
- **Jonathan Gerszberg** (University of Michigan)
- **Sanchari Ghosh** (Dartmouth College)
- **Joshua Pajak** (University of California-San Diego)
- **Ingrid Paredes** (New York University)
- **Hossain Shadman** (University of Delaware)
- **Elliot Taylor** (Tufts University)
- **Xinyang Yin** (Penn State University)

Satvik Sharma, a master’s student was selected as a New Jersey Space Grant Consortium fellow for the 2015-2016 year. His work focuses on studying chemical binding interactions in both normal and microgravity environments. ■



Eric Jaycock Earns Distinguished Young Alumnus Award at 2015 Medal of Excellence Event

CBE alumnus, **Eric Jaycock**, Ph.D. GSNB’04, GSNB’11, received the School of Engineering’s 2015 Distinguished Young Alumnus Award, which was presented in October at the annual Medal of Excellence dinner. Each year the school recognizes alumni for their achievements in industry, research, and service. Jaycock is the director of continuous manufacturing at Patheon, a leading provider of drug substance and product services for the global biopharmaceutical industry. While at Rutgers he earned his doctoral degree under the direction of Prof. Fernando Muzzio and contributed to the development of scalable manufacturing processes for oral solid dosages as part of the NSF Engineering Research Center for Structured Organic Particulate Systems (C-SOPS) and in conjunction with Janssen Pharmaceuticals, Inc.

Shishir Chundawat Part of Team Characterizing Critical Biofuel Enzymes Using Single-Molecule Techniques

Making fuel from plants has long been a goal of scientists and engineers hoping to tame wild swings in fuel prices and availability and to ultimately prepare for a time when finite supplies of petroleum dry up.

But the promise of obtaining abundant and sustainable supplies of liquid fuel from biomass - by-and-large agricultural crops - is a challenge that still vexes scientists and engineers after decades of research.

Rutgers School of Engineering assistant professor Shishir Chundawat, who joined the Chemical and Biochemical Engineering faculty in 2015, is one of the experts taking up the challenge.

"One of the big drivers for the work I do - and it's my personal philosophy also - is that it's important to be sustainable," he said, "Having sustainable ways to produce energy would allow society to deal with many of the issues we face."

Plant biomass, he notes, is theoretically self-sustaining. "It can essentially grow with just the availability of carbon dioxide, water and sunlight."



Yet achieving this sustainability is not straightforward. Ethanol, a popular additive that stretches gasoline supplies and cuts pollution, is made from corn grain, but its production requires a lot of energy input - mainly for the fertilizer used to grow the corn. It also demands high-quality land that could otherwise be used for food crops.

However, grasses and woody plants such as switchgrass and poplar grow abundantly on land not suited for food crops and with little upfront energy input. They store a lot of energy as carbohydrates, but unlike with cereal grains



Prof. Chundawat (pictured above left with students and below) began looking at converting inedible biomass to value-added products early in his undergraduate research and into his postdoctoral studies with the Great Lakes Bioenergy Research Center, funded by the U. S. Department of Energy.

and seeds, those carbohydrates are not easy to 'press out' and process into simple sugars - the building blocks for fuels and chemicals. Grass and wood carbohydrates are locked into plant structures such as plant cell walls as long-chain cross-linked polymers.

Of the nearly 16 billion gallons of ethanol produced annually in the United States, nearly all comes from corn grain. Only a few hundred million gallons come from cellulosic inedible biomass. The Department of Energy is targeting sufficient cellulosic biofuel production by 2030 to replace nearly 30 percent of the country's current petroleum consumption.

"The growth in cellulosic biofuels seems to be slow and steady," he said, "but there are both logistical and scientific issues that have to be sorted out."

Chundawat and other scientists are attacking the problem biologically - searching for enzymes that break down this tightly bound biomass into simple sugars. By examining the synthesis and breakdown of sugar polymers at the cellular level, they are looking for enzymes suitable for large-scale industrial processes.

Chundawat says he's in good company at Rutgers, citing colleagues in his department such as Fuat Celik and George Tsilomeliekis doing work on chemical catalysis to upgrade

plant biomass to useful products, and Haoran Zhang who is engineering microbes to make fuels and chemicals. He also sees opportunities for collaboration in other Rutgers schools and centers.

But beyond merely looking for enzymes that can do the job, Chundawat is looking to engineer and characterize new enzymes that are more effective. He is currently a co-PI on a National Science Foundation award to understand and engineer enzymes to reduce non-productive enzyme binding to lignin polymers present in biomass during biofuel production.

"The problem is that enzymes get stuck on biomass," he said. "We are essentially trying to understand how to overcome that barrier." He believes using protein engineering to make novel enzyme mutants and characterizing their activity with new analytical tools will shed light on the problem. He recently also won the 2016 Ralph E. Powe Junior Faculty Enhancement Award from the Oak Ridge Associated Universities to develop low-cost pretreatments and biological processes for converting waste cellulosic biomass into fermentable sugars. ■



To see a complete list of honorees, for more information, or to purchase tickets, visit: www.soe.rutgers.edu/moe2016.

2016 Medal of Excellence Honorees Announced

*Rutgers School of Engineering
Medal of Excellence Awards Dinner
Thursday, October 13, 2016
Livingston Student Center
Rutgers University-New Brunswick*

*6:00 p.m. Cocktail Reception
7:00 p.m. Dinner and Program*

Of the six Rutgers University School of Engineering alumni to be recognized for their professional accomplishments and contributions at the annual Medal of Excellence and Distinguished Alumni awards dinner, two are from the Department of Chemical and Biochemical Engineering.

The Medal of Excellence, which honors alumni whose superior achievements have honorably reflected the School over the course of his or her lifetime, will be presented to **Marvin Schlanger**. Graduating in 1969 with a bach-

elor's degree, Schlanger is the former chief operating officer, president and chief executive officer of ARCO Chemical. During his career he has received the American Institute of Chemical Engineers' Lifetime Achievement Award and the NPRA Petrochemical Heritage Award. He has written multiple papers based on his research, and his expertise has been called on by the United States Congress.

The Distinguished Achievement in Industry award will be presented to **Vijay Swarup**, Ph.D. who is the vice president for research and development at Exxon Mobil Research and Engineering Company. Swarup earned both his master's and doctoral degrees from Rutgers in 1988 and 2000, respectively. Swarup will be recognized for his contributions toward creating more efficient and cleaner fuels and other innovative technologies. Part of his research extends into using algae to produce biofuels, rather than the more traditional ethanol fuels.

Photography: Dennis Connors, Don Hamerman, Keith Muccilli

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School of Engineering

The Department of Chemical and Biochemical Engineering
Rutgers, The State University of New Jersey
98 Brett Road
Piscataway, NJ 08854-8058

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