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COLUMNS

CHEMICAL AND BIOMOLECULAR ENGINEERING

A. JAMES CLARK SCHOOL of ENGINEERING

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A NEWSLETTER FOR ALUMNI AND FRIENDS OF THE DEPARTMENT OF CHEMICAL AND BIOMOLECULAR ENGINEERING AT THE A. JAMES CLARK SCHOOL OF ENGINEERING, UNIVERSITY OF MARYLAND.

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Anisimov Group Seeks Critical Point of Supercooled Water

Water is one of the most familiar substances on earth, but still keeps some secrets. Department of Chemical and Biomolecular Engineering (ChBE) and Institute for Physical Science & Technology (IPST) Professor **Mikhail Anisimov** and his research group are out to discover them.

The team has received an American Chemical Society Petroleum Research Fund Grant for a proposal titled "Cold Water: A Novel Supercritical-Fluid Solvent." The project will explore the unusual properties of supercooled water, which remains in a liquid form well below 0 °C (32 °F).

A critical point is a temperature at and beyond which multiple phases of water (such as fluid and vapor) cease to exist and the water becomes what is known as a supercritical fluid. Near these critical points, fluids possess unusual properties, such as high compressibility and very low interfacial tension.

While the high-temperature vapor/liquid critical point of water and the phenomena surrounding it are known and

have been well studied, whether a liquid/liquid critical point exists at very cold temperatures has not been clearly established and has been debated since the mid-1990s. Anisimov and his group hope to find that critical point, which could confirm whether or not water becomes polyamorphous (capable of existing in multiple liquid forms), and could pave the way for the use of cold water as a supercritical fluid solvent.

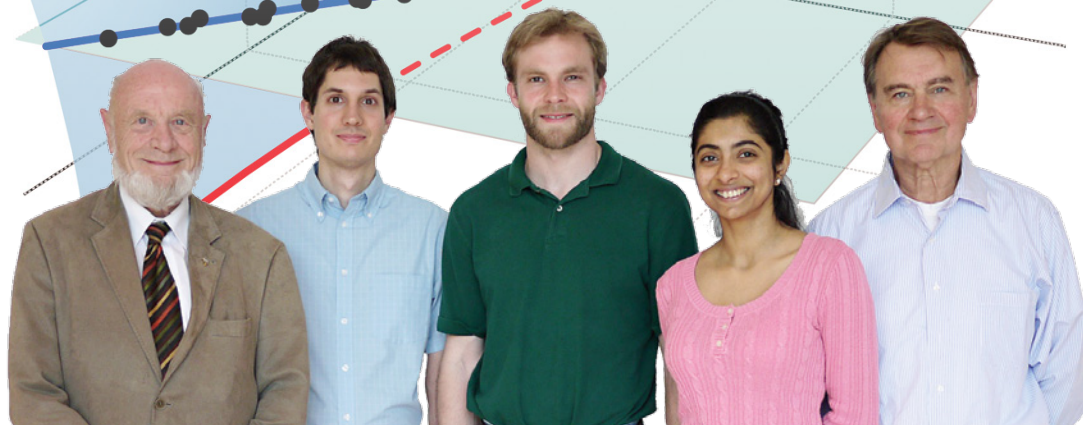
Previous studies (e.g., Stanley *et al.* 2008) have hypothesized that if water can exist in two forms at a liquid/liquid critical point, one would be similar to ordinary liquid water, while the other would be a low-density liquid with a density similar to that of ice.

"Small samples of very pure liquid water can be supercooled down to about -38 °C [-36 °F], where they freeze to ice," explains Anisimov Group member and ChBE research scientist Dr. **Vincent Holten**. "Measurements on supercooled water show that several properties, such as heat capacity

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BACKGROUND IMAGE: PRESSURE-TEMPERATURE-CONCENTRATION GRAPH OF SUPERCOOLED WATER.

LEFT TO RIGHT: PROFESSOR EMERITUS JAN V. SENGERS, DR. VINCENT HOLTEN, JOHN BIDDLE, DR. DEEPA SUBRAMANIAN, AND PROFESSOR MIKHAIL ANISIMOV.





SHERYL EHRLMAN

GREETINGS TO ALUMNI AND FRIENDS OF CHEMICAL AND BIOMOLECULAR ENGINEERING AT THE UNIVERSITY OF MARYLAND!

I take a shuttle bus from the Metro to campus most days, and it's hard not to notice the University's "Fearless..." campaign (see <http://ter.ps/fearless>), which appears in advertisements on the shuttle, as well as in other locations around the College Park campus. How does the word "fearless" apply to Chemical and Biomolecular Engineering? How about fearless graduate students **Chanda Arya** and **Kevin Diehn** from Professor **Srini Raghavan's** group,

who have recently started a company with support from the Maryland Industrial Partnerships Program? Or our recent Ph.D. graduate **Deepa Subramanian** and her advisor **Mikhail Anisimov**, who received a grant from the National Science Foundation ICorps program to promote commercialization of their work on small molecule aggregation? Or our fearless undergraduate student and Boren Scholar **Lisa Wiest**, who is finishing up her exchange year at Yonsei University in Korea? Or our Chem-E car team, which headed to Rutgers to compete at the mid-Atlantic regional competition, again building batteries from scratch, and once again qualifying for the national competition this fall?

Fearless also describes the increasing numbers of first year and transfer students who decide to major in chemical engineering, and the increasing number of M.S. and Ph.D. students in our graduate program. Chemical engineering is still one of the toughest programs around, but the opportunities afforded by the degree keep drawing students in. While they are here, they are participating in study abroad, entrepreneurship and undergraduate research programs. Our fearless faculty and staff are meeting the challenge associated with these rising enrollments, working harder than ever to maintain a high quality educational experience for our students and to produce important scholarly advances.

More fearless ChBE stories are inside this newsletter and you can always stay up to date by visiting our web site at www.chbe.umd.edu/news.

Go Terps!

Sheryl H. Ehrman
Keystone Professor and Chair

ANISIMOV GROUP continued from page 1

and compressibility, exhibit a strong increase with cooling, which looks similar to the behavior near a critical point." But, he says, these behavioral anomalies are difficult to study. "If this critical point exists, it would be located at a temperature where liquid water cannot exist, making it experimentally inaccessible."

The group's approach is to add a solute, such as a salt or alcohol, to samples of pure, supercooled water. This should raise its critical point to higher temperatures, making it observable through experimental, theoretical, and computational investigations.

In addition to Anisimov and Holten, past and present investigators include graduate student **John Biddle** (Department of Physics), alumna **Daphne Fuentevilla** (M.S. '07, Ph.D. '12), ChBE research associate Dr. **Deepa Subramanian** (Ph.D. '12), and Princeton University professor **Pablo G. Debenedetti**. ChBE and IPST Distinguished University Professor Emeritus **Jan Sengers** is collaborating with the team.

INSTRUMENTATION AWARDS FOR SPRAY CHARACTERIZATION, SMALL ANGLE X-RAY SCATTERING

ChBE professors are among the recipients of two National Science Foundation Major Research Instrumentation Grants recently awarded to the Clark School.

Associate Professor **Andre Marshall** (joint; Fire Protection Engineering and Aerospace Engineering) ChBE professor and chair **Sheryl Ehrman** have received \$376,892 in funding for a proposal titled "MRI: Development of Spatially-resolved spray scanning system." Their team seeks to design an instrument capable of precisely characterizing engineered sprays in order to develop models to describe their behavior and to leverage this understanding for advancements in spray technology. They are focusing on both large-scale sprays, such as those used in fire suppression applications, and small-scale sprays, such as those used in microelectronic applications. Ehrman will serve as the project's co-PI.

ChBE professor **Srinivasa Raghavan** is one of several co-PIs on a team that has received \$345,800 in funding for its proposal, "MRI: Acquisition of a Small Angle X-Ray Scattering System for the Characterization of Nanoscale Structures." The award will allow for the purchase of a Small Angle X-ray Scattering (SAXS) system for the characterization of nanoscale structures in materials. Nanoscale characterization is a critical step in the design of new materials for applications in areas as diverse as energy, microelectronics, civil infrastructure, defense and health and for the understanding of the basic science underlying these applications. The new instrument will anchor a state-of-the-art facility designed to serve the nano- and biosciences research and education needs of both the campus and the region. Professor and chair **Robert M. Briber** (Department of Materials Science and Engineering) is the project's P.I.

ALL-IN-ONE: \$300K FOR DEVELOPMENT OF INTERFACE-FREE BATTERY

ChBE and University of Maryland Energy Research Center associate professor **Chunsheng Wang** has spent the past several years focused on building the next generation of smaller and more powerful lithium-ion batteries, developing new electroanalytical techniques, high surface area electrodes built on a virus, and a fracture-resistant silicon anode. Now, he's rethinking the battery's fundamental structure. Backed by a three-year, \$300,000 single-PI grant from the National Science Foundation's Division of Chemical, Bioengineering, Environmental, and Transport Systems, Wang is set to pursue the creation of all-solid state, interface-free lithium-ion batteries.

Current solid-state lithium-ion batteries use three different materials for their anodes, cathodes, and electrolytes, creating resistance at the interfaces between the electrolytes and electrodes. This resistance is a significant cause of low power density, lower energy output, and reduced battery lifecycles—factors that not only prevent lithium-ion batteries from becoming feasible for use in high power electronic devices, but also keep them larger in size. Wang is working on the fabrication of a “single continuous phase” material that would encompass the anode, electrolyte, and cathode. Free of the traditional material interfaces, the new battery would have more power, operate more efficiently and safely in high temperatures, and could be reduced to nanoscale dimensions to power microelectromechanical systems.

The project will explore the effects of interface properties on existing batteries, study the formation mechanisms of interface-free batteries, and discover the performance, structure and composition of materials that could be used in the fabrication of high-temperature, interface-free solid-state lithium-ion batteries.

Wang believes that if the work is successful, the new batteries will have a profound impact on the automotive, electronics, and renewable energy industries.

LIU: ACS PETROLEUM FUND GRANT

ChBE assistant professor **Dongxia Liu** has been awarded a 2-year grant from the American Chemical Society's Petroleum Research Fund to develop a new technique for transforming heavy carbon-based energy resources into clean fuels.

“Emerging sources of carbon-based fuels, such as biomass, coal, and tar-sands, are substantially heavier than conventional crude oil, and contain higher proportions of heteroatoms such as sulfur, nitrogen, and oxygen,” Liu explains. “We propose to develop novel structured catalysts to enable effective and selective catalytic reactions for processing of these heavier fuel feedstocks into clean fuels.”

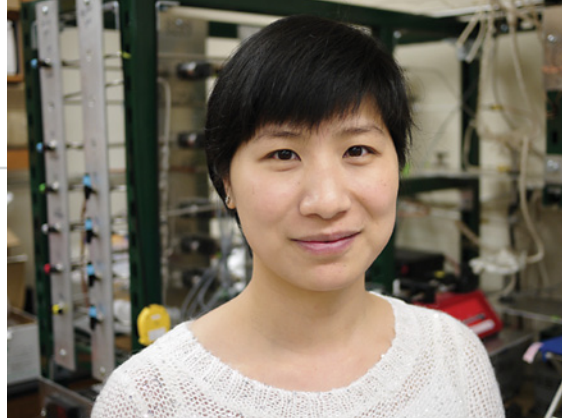
The project based on Liu's proposal, “Metal Sequestered in Hierarchical Zeolites: Protected Active Sites and Enhanced Mass Transport for Heteroatom-Tolerant Catalysts,” will combine metal and zeolite bifunctional catalysts into novel porous nanoarchitectures capable of removing heteroatoms from heteroatom-containing compounds in the feedstocks while minimizing the formation of coke on the catalyst.

According to Liu, the structural and chemical characterization and kinetic analysis of the new catalyst formulations and the catalyzed reactions will also provide fundamental information about the relationship between catalyst structure and functionality, which should guide the development and application of other efficient fuel-processing catalysts.

MARYLAND HOSTS MID-ATLANTIC SOFT MATTER WORKSHOP

Researchers from throughout the region interested in all things “soft and squishy” gathered to share their ideas at the ninth Mid-Atlantic Soft Matter Workshop (MASM 9), held on the University of Maryland, College Park campus in 2012. The event provided a casual forum for students, faculty and staff from academia, industry and national laboratories to present their latest results, network, and seek out new collaborations.

A wealth of materials can be classified as “soft matter,” including polymers, films, liquid crystals, emulsions, gels, self-assembled



DONGXIA LIU

structures and systems, cells, tissue, and biomimetic materials. Researchers in the field may be engaged in soft matter's creation, behavioral simulation, manipulation, interfacial properties, biophysics, rheology and hydrodynamics, and replication.

The workshop's goal is to highlight the ways in which scientists from a variety of disciplines—including engineering, biology, chemistry, and physics—approach the study of soft materials and use them in their research. MASM demonstrates how, through a shared interest in soft materials, scientists can discover that their fields and interests may overlap in unexpected ways.

Presentations included formal talks given by invited soft matter experts from regional institutions including Johns Hopkins University, Penn State, the University of Delaware, the University of Maryland, and the University of Pennsylvania. The program also included over 30 three-minute “sound bites,” project overviews delivered by undergraduates, graduate students, and postdoctoral research associates.

Clark School professors **Robert M. Briber** (chair, Department of Materials Science and Engineering) and **Srinivasa R. Raghavan** (Department of Chemical and Biomolecular Engineering), College of Mathematical and Natural Sciences professor **Wolfgang Losert** (Department of Physics) and Georgetown University professor **Daniel Blair** (Department of Physics) organized the event, which had 110 registrants from across the mid-Atlantic region.

Support for MASM 9 was provided by the Clark School's Departments of Chemical & Biomolecular Engineering and Materials Science & Engineering, the University of Maryland—National Cancer Institute Partnership for Cancer Technology, and Georgetown University's Institute for Soft Matter Synthesis and Metrology.

HYBRID GELS:

A) A MESSAGE IS WRITTEN WITH THE FIRST LIQUID PRE-GEL, THICKENED WITH LAPONITE CLAY PARTICLES, ON A PETRI DISH, AND THE SECOND IS POURED AROUND IT.

B) AFTER POLYMERIZATION, THE RESULT IS A SINGLE, CLEAR GEL.

C) THE AREA CONTAINING LAPONITE PARTICLES REFRACT POLARIZED LIGHT DIFFERENTLY THAN THOSE THAT DON'T, REVEALING THE MESSAGE.

D) IN A SIMILAR EXPERIMENT, THE OUTER GEL WAS HEAT SENSITIVE. THE LAPONITE-LACED GEL WAS NOT, AND REMAINED CLEAR WHEN HEATED, REVEALING THE MESSAGE.

E) HYBRID GELS MADE BY POLYMERIZING ONE, POURING IN A SECOND, AND THEN POLYMERIZING IT, RESULT IN A WEAK BOND BETWEEN THE LAYERS.

F) THE RAGHAVAN GROUP'S TECHNIQUE RESULTS IN A STRONG BOND WITH VERY LITTLE MIXING OF THE TWO PRE-GELS. IN THIS EXAMPLE, THE HYBRID GEL DOES NOT TEAR AT THE JUNCTION WHEN STRETCHED, AND IT EXHIBITS TWO DIFFERENT MECHANICAL PROPERTIES: THE BLUE SIDE, A PHYSICALLY CROSSLINKED POLYMER, IS MORE FLEXIBLE THAN THE GREEN SIDE, A CHEMICALLY CROSSLINKED POLYMER.

THE GEL WITH THE SECRET CENTER

A new "hybrid gel" created by the Complex Fluids and Nanomaterials Group has certainly earned its "smart material" title. In a single sample, the multi-talented goo's chemical, mechanical and optical properties can change from one sometimes visually indistinguishable zone to another. It can even carry secret messages.

The group, led by the lab's director, ChBE professor and associate chair **Srinivasa Raghavan**, recently published a paper describing the gel in *Macromolecules*. The work was also featured in the *New Scientist's* "One Per Cent" column.

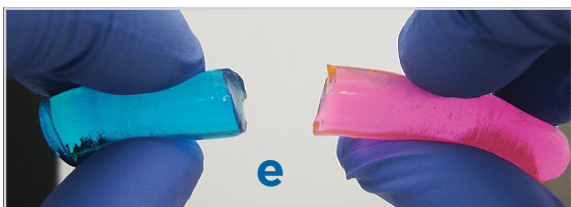
The Raghavan Group isn't the first to combine gels with different properties, but

team members believe they are the first to overcome a significant obstacle to doing it well.

"People have tried layering different gels together by polymerizing the first, layering the second in its liquid pre-gel state on top, then polymerizing that one, and so on, sort of like layering Jell-O," explains **Stephen Banik** (M.S. '12), who first-authored the paper and wrote his thesis on the gel. "The problem is the layers are only weakly hooked together where they interface. If you apply just a little bit of stress to them, they come apart." (See fig. e, below.)

The key to creating strong bonds, he says, is to polymerize two or more liquid pre-gels at the same time, allowing them to interpolymerize across an interface. The challenge is to do it without allowing the pre-gels to mix.

The secret of his gels' success is Laponite®, an inorganic clay used to control the viscosity of many water-based products such as paint and cosmetics. Banik found he could put two liquid pre-gels next to or on top of each and polymerize them simultaneously, without mixing, as long as one of them had been thickened with Laponite. The difference in viscosity allowed each material to retain its special properties while gelling and bonding. The result was a single, rugged gel that did not tear apart or rupture where the two zones met.



Banik created two kinds of gels that revealed hidden messages inside under different circumstances. In both cases he used cake-decorating bags to write the letters “UMD” in a Laponite-thickened pre-gel on a shallow dish (*see fig. a*). He then carefully poured a second, liquid pre-gel around it. The first pre-gel’s thickness prevented it from dissolving into the second, like a line of toothpaste surrounded by water. After polymerization, the dish appeared to contain a single, clear gel (*see fig. b*), but different areas responded to different stimuli.

One sample, when heated, turned opaque where the second pre-gel had been poured, revealing the message as clear letters (*see fig. d*). The other’s zones had different optical properties: the Laponite particles in the initials “UMD” refracted polarized light differently than the gel around it, making them visible (*see fig. c*).

The same technique was also used to make hybrid gels containing different levels of flexibility, ones that shrank and expanded as they retained and lost water at different rates, and ones that selectively absorbed dyes (*see fig. f*).

With additional development, hybrid gels like these could be used in industrial or biomedical products. Potential applications include coatings that respond to changes in temperature, conditional or extended release capsules for drugs, biomimetic devices, tissue engineering, and optical computing.

RUEGER: MIXING FORUM AWARD

ChBE graduate student **Paul Rueger**, advised by Professor **Richard V. Calabrese**, won the 2012 North American Mixing Forum (NAMF) Student Award for a paper titled “Dilute Dispersion of Water into Oil in a Batch Rotor-Stator Mixer.” Rueger received the award and presented the paper at the Mixing 23 conference held in Cancun, Mexico in 2012.

Rueger’s work focuses on rotor-stator mixers, which are used to produce emulsions, materials consisting of one insoluble liquid dispersed as microscopic droplets within another liquid. (The oil and vinegar mixture shaken to create salad dressing is

perhaps the best-known example.) As droplets of the dispersed liquid are moved around their surrounding liquid by the mixer, they encounter high levels of shear stress, which cause them to break apart into even smaller droplets. For dilute concentrations of the droplet phase, eventually the emulsion reaches its ultimate drop size distribution, a quantifiable, final degree to which one liquid can be dispersed into another liquid for a specific set of conditions.

“It’s desirable to know what conditions are required to obtain which drop size distributions in industrial settings,” Rueger explains. “That way we can accurately predict what to expect without the need to run those experiments in a plant, which would be very costly. Drop size distribution depends on things such as the rotor speed, the rotor-stator dimensions, the interfacial tension between the two liquids, and the viscosities of the two liquids. My goal is to develop expressions that will allow small-scale lab experiments to accurately predict the ultimate drop size distributions in large-scale systems with similar physical properties and experimental conditions.”

While predictive mathematical models have been developed for systems where the continuous phase is a low viscosity liquid such as water, less information is currently available when it is a high-viscosity liquid like oil. Inside a rotor-stator mixer, the flow of low viscosity liquids is usually turbulent (chaotic), but thicker fluids may exhibit either a turbulent or laminar (orderly) flow.

Rueger’s work expands on our ability to predict droplet size in high viscosity emulsions under both flow conditions. For turbulent flow, his study expanded the range of physical properties under which a previously known turbulent correlation has



PAST AND CURRENT MEMBERS OF THE CALABRESE GROUP AT NAMF 2012. LEFT TO RIGHT: **JUSTIN R. WALKER** (PH.D. '12), **GUSTAVO A. PADRON** (M.S. '01, PH.D. '05), PROFESSOR **RICHARD V. CALABRESE**, AND THIS YEAR'S NAMF STUDENT AWARD WINNER, **PAUL E. RUEGER**. WALKER AND PADRON HAVE ALSO WON THE AWARD.

been experimentally verified. For laminar flow, his study provides an empirical correlation and, by comparison with previous work, discovered the mechanism by which drops break up.

Rueger says that the new information could be beneficial in various contexts such as deep-sea oil drilling. At low temperatures and high pressures, methane hydrate gas dispersed in oil can freeze into masses capable of clogging pipes and pumps. Using these types of models and performing small-scale laboratory experiments, petroleum engineers can make predictions about how strong the shear fields in the pipeline have to be in order to break up the frozen particles sufficiently for them to pass through.

Rueger is the third member of the Calabrese Group to win the NAMF Student Award, which has been given only six times since 1997. **Justin Walker** (Ph. D. '12) won the award in 2010, **Gustavo Padron** (M.S. '01, Ph.D. '05) won in 2005, and two other group members, **Karl Kevala** (M.S. '01) and **Supathorn Phongikaroon** (Ph.D. '01), were finalists in 2003 and 2001, respectively.

“I am, of course, pleased to have won,” Rueger tells us, “but I’d also like to point out that the fact that Professor Calabrese’s students keep winning this contest shows everyone what I already knew: He really is an excellent advisor!”

DOMINION RESOURCES SUPPORTS LAB UPGRADE

The Clark School's Department of Chemical and Biomolecular Engineering's (ChBE) primary teaching lab will soon host a new piece of core equipment thanks to a gift from Dominion Resources, one of the nation's largest

producers and suppliers of electricity and natural gas.

The Dominion Foundation awarded ChBE a \$30,000 grant to fund the purchase of a new heat exchanger system for the department's Unit Operations Lab, where all students majoring in chemical



STUDENTS AND FACULTY IN THE UNIT OPERATIONS LABORATORY WITH MARK REASER, DIRECTOR OF OPERATIONS AT DOMINION'S COVE POINT LNG TERMINAL (CENTER, HOLDING CHECK).

engineering learn to use and manage the pilot plant apparatus and facilities they will encounter in the field. In a ceremony held in the lab in September 2012, **Mark Reaser**, director of operations at Dominion's Cove Point LNG Terminal in southern Maryland, presented ChBE professor and chair **Sheryl Ehrman** with the check.

6

The department's existing heat exchanger station, which is used to demonstrate heat transfer from one medium to another, was hand-built more than 15 years ago and is completely manual in operation. The new computer-controlled instrument, from Armfield, is an educational system designed to allow students to experiment with hot and cold fluids, visualize fundamental concepts, test process control strategies and record data.

"The experiment lets the students see how the theory of heat transfer that they learned in transport [class] is applied to an actual piece of equipment," explained Assistant Professor **Amy Karlsson**, who co-teaches the unit operations course. "They can run the system using different configurations and see how their experiment results compare with theoretical calculations." She added that the new exchanger will help modernize the lab.

Ehrman explained to the assembled guests that the new heat exchanger would have impact beyond the senior-level course in which it is most commonly used. "We want to use this new station, along with a few other changes we'll be making to the lab, as a way to show elementary, middle and high school students who come to campus for open houses and summer camps, on a small scale, what chemical engineers do," she said. "This is a great way to demonstrate chemical engineering in action."

"I appreciate the opportunity to present this contribution to the project here today on behalf of the Dominion Foundation," Reaser said, adding that since 1996, the company has bestowed over \$3 million in science-, math-, education-, and outreach-related grants.

The Clark School's Associate Dean for Faculty Affairs and Graduate Programs, Professor **Peter Kofinas** (Fischell Department of Bioengineering), thanked the Dominion Foundation at the ceremony. "We're really excited about Dominion's investment in our students," he said, "and we're really looking forward to a lasting relationship."

WHERE CHEMICAL ENGINEERING AND GREEN THUMBS MEET

What does chemical and biomolecular engineering have to do with plant biology and metabolism? If you want to understand



LAUREN DORSEY

how to turn crops or trees into the raw ingredients of sustainable fuels and biodegradable plastics and fabrics, the answer is "quite a lot, actually!"

ChBE junior **Lauren Dorsey**, advised by Assistant

Professor **Ganesh Sriram**, has received a Howard Hughes Medical Institute (HHMI) undergraduate research fellowship to support her efforts to understand how poplar trees (also known as cottonwood or aspen) store and recycle nitrogen, an important nutrient. What she learns could help improve the resilience of agricultural crops and help engineer other plants for use in sustainable biofuel or chemical production.

The competitive HHMI Fellowship program, co-sponsored by HHMI and the University of Maryland's College of Computer, Mathematical, and Natural Sciences, supports the research activities of undergraduates interested in pursuing careers in medical, biological or life sciences. The program's goals are to immerse students in the investigative process, increase their aptitude for research, and provide them with the opportunity to collaborate directly with a faculty mentor.

Dorsey has worked in Sriram's Metabolic Engineering Laboratory since the fall of her sophomore year. She contributes to the group's goal of determining how poplar can be modified into a high-yield, cost-effective and renewable biofuel crop, but her focus on how it processes nitrogen could have far-reaching benefits.

"When nitrogen is depleted, plants' photosynthesis and respiration are reduced, which can lead to increased mortality," she explains. "Nitrogen helps plants resist environmental stresses from disease and drought. Poplar trees are particularly adept at

storing and recycling nitrogen, so it's a great model organism to study."

Understanding how plants store and recycle nitrogen, and how to improve their ability to do so, could lead to healthier societies and the development of more sustainable resources. Crops that suffer from nitrogen depletion during droughts could be generically engineered to retain it, allowing them to survive. They may also require less nitrogen-rich fertilizer, which is both expensive and potentially hazardous to the environment. Plants with little or no commercial value could be converted into high-yield biomass crops that provide the ingredients for sustainable and biodegradable products usually made from petroleum, such as fuels, plastics, and synthetic fabrics.

Dorsey uses a technique called metabolic flux analysis to track and map how and where nitrogen is metabolized. She gives her poplars food "labeled" with a nitrogen isotope called ^{15}N , a nitrogen atom containing one extra neutron, which can be detected by a device called a mass spectrometer. She also analyzes the amount and location of a protein called BSP, which is used to store nitrogen. She varies the amount of nitrogen-rich food she gives the plants to determine the effect it has on where the nitrogen is routed and stored, and on how fast it happens.

While much of the Sriram Group's prior research has examined activity at the cellular level, Dorsey is working with poplar plants, a move expected to provide more accurate data about its behavior. "In previous experiments, we thought that whatever happens in our tree is going to happen in each cell," she says. "But isolated cells do not necessarily represent what's going on in different regions, like the bark vs. the leaves." Before turning to the whole plant, she says, the lack of a "big picture" network also left them unable to track BSP.

Dorsey isn't surprised when people ask whether her work seems more like something a biologist would do—even she joined the Sriram Group because she was interested in biofuels, but hadn't thought about the inner workings of the plants they come from.

"I like to think of it as using [what] we learn in our classes for other purposes,"

she says. "In Kinetics, we studied how reactions proceed—what makes them faster or slower. That's a basic chemical engineering technique. In the Sriram Group, we're applying it to biology." Chemical and biomolecular engineers, she adds, think about biological problems in a different way, particularly because their drive to solve a biological mystery lies in wanting to apply it to a greater problem, like overcoming our dependency on oil. "[We're] trying to solve a problem in a more interdisciplinary way."

Participating in undergraduate research has had a very positive effect on both Dorsey's Clark School experience and her future plans. As a freshman, she wasn't sure what she wanted to do or whether she should major in chemical engineering, but her work in the lab helped her decide that she's in the right place.

"I've found I really like doing research," she says, adding that she's now considering pursuing a graduate degree. "It's one of the best things an undergrad could do to increase their understanding of their classes and their overall interest in engineering."

CHEM-E CAR AT AICHE

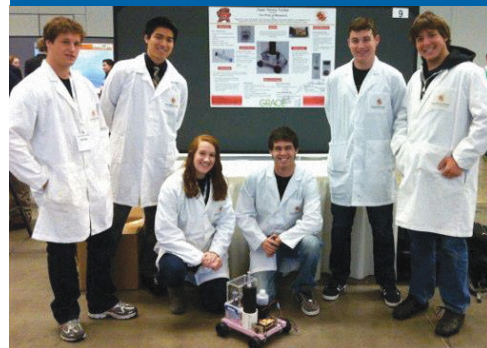
The model car known as *The Pride of Maryland* stopped within two meters of the finish line at the 2012 Chem-E Car finals, not much farther off than the performance that had earned its team, the Thirsty Turtles, a second place win at the regional competition.

But *The Pride of Maryland* had company. A third of the cars in the competition, held at the national meeting of the American Institute of Chemical Engineers (AIChE) in October, also finished within two meters of the finish line, creating a fight for the top spots. When it was all over, the Thirsty Turtles stood in 11th place, and finished 2nd in the event's poster competition.

The results aren't a disappointment to the relatively young team, which fielded its second car in as many years and found itself up against seasoned opponents.

"We are proud of ourselves and our car," says ChBE senior and Thirsty Turtles team member **Amy Nutis**. "The 2012 National Chem-E Car competition was very intense, with

MEMBERS OF TEAM THIRSTY TURTLES AT THE AICHE CHEM-E CAR FINALS IN PITTSBURGH, PENN. IN OCTOBER 2012. LEFT TO RIGHT: NICHOLAS LEPAK (SENIOR), WESLEY YAN (SENIOR), AMY NUTIS (SENIOR), ISAAC ZAYDENS (SOPHOMORE), TRAE VANASKEY (SOPHOMORE), AND MATTHEW FORD (SENIOR, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING).

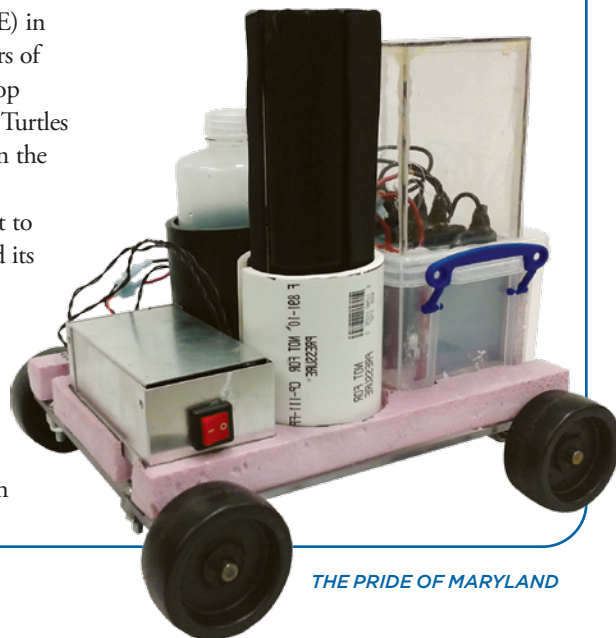


the top teams coming within centimeters of the line and the first place finisher landing perfectly on it... We learned a lot from the other teams... as well as what worked and didn't work from our car's performance. We are all really excited to start fresh and begin designing our new car!"

The AIChE's Chem-E Car contest challenges teams of students to design and construct a small, chemically powered model vehicle. The cars must carry a specified cargo over a distance only revealed at the competition, and stop as close to a finish line as possible. Any kind of chemical reaction may be used to power the cars, which are not remote-controlled. Each team must carefully calculate the duration of the reaction required when they are told how far their vehicle must travel.

This year, AIChE officials announced a target distance of 21 meters and a payload of 300mg at the finals. *The Pride of Maryland*

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E. A. (Ed) Clerke (MS '78 and Ph.D. '82, physics), formerly advised by ChBE Distinguished University Professor Emeritus **Jan Sengers**, was named the Principal Professional of the Reservoir Characterization Department and Exploration at Saudi Aramco, the highest technical position in the company. Clerke is known for his innovations in techniques used to unlock and characterize subsurface reservoir carbonate fields for ultimate oil and gas recovery.

Hyunmin Yi (Ph.D. '03, chemical engineering) has been promoted to Associate Professor in the Department of Chemical and Biological Engineering at Tufts University. At Maryland, Yi was advised by Fischell Department of Bioengineering professor and chair **William E. Bentley**, and later worked as a postdoctoral research associate for Department of Materials Science and Engineering professor **Gary Rubloff**.

John March (Ph.D. '05, chemical engineering), formerly advised by BioE Professor and Chair **William E. Bentley**, has been promoted to Associate Professor with tenure in the Department of Biological and Environmental Engineering at Cornell University.

recent DISSERTATIONS

DECEMBER 2012

Aaron Fisher: "Polymer-Ionic Liquid Hybrid Electrolytes for Lithium Batteries." Advisor: **Peter Kofinas** (Fischell Department of Bioengineering)

Daphne Fuentevilla: "Hot and Cold Water as a Supercritical Solvent." Advisor: **Mikhail Anisimov**

Shilpa Nargund: Mapping Metabolic Fluxes in Plant Cells to Understand Carbon-Nitrogen Interactions and Nitrogen Storage and Cycling. Advisor: **Ganesh Sriram**

Kai Zhong: "Co-Solvent Assisted Spray Pyrolysis for the Preparation of Metal Microparticles." Advisor: **Sheryl Ehrman**

CHEM-E CAR, continued from page 7

traveled 22.97 meters. Cornell University's car took first place, while the University of Puerto Rico and Oklahoma State University came in second and third, respectively.

The Pride of Maryland is built on a bi-axial chassis with a four-wheeled frame, and uses a direct drive motor attached to the underside of its top deck. The car is powered by a zinc-air fuel cell battery, which contains six cells connected in series, using zinc as the anode, a specially coated membrane as the separator, and sodium hydroxide as the electrolyte. An iodine photochemical reaction, which detects an absence of light from an LED using photoresistors in the reaction chamber, is used to stop the vehicle. In addition to Nutis, Team Thirsty Turtles includes ChBE undergraduates **Yousif Alsaid, Richard Grave, Nick Lepak, Lenny Pagliaro, Katie Pohida, David Shoemaker, Trae Vanaskey, Wesley Yan, and Isaac Zaydens**; and **Matthew Ford** from the Department of Electrical and Computer Engineering. The team is advised by ChBE associate professor **Chunsheng Wang** and sponsored by the W.R. Grace Foundation.

BOREN LANGUAGE SCHOLAR PURSUES RESEARCH, CULTURAL STUDIES IN KOREA

Last issue we told you about ChBE sophomore **Lisa Wiest**, who was awarded the U.S. Department of Defense's prestigious Boren Language Scholarship to spend the 2012-2013 academic year studying Korean at Yonsei University in Seoul, South Korea. We checked in with her over the Korean Lunar New Year holiday in early 2013 to find out how she spent her first semester abroad.

In the fall, Wiest took courses in biochemistry and Korean language and culture. Thanks to connections made through her advisor, ChBE professor **Kyu Yong Choi**, she has also joined Yonsei University professor **Il Moon's** research group, which focuses on process systems engineering. In the lab, Wiest has been learning software applications used in computational fluid dynamics, and has been working with some of the team's graduate students on the development of a model of part of the residue fluidized catalytic cracking process. She plans on taking a course in reaction engineering—the equivalent of ChBE's kinetics course—in the spring.

Wiest says the informal learning that comes with a study abroad experience has been even more valuable than what she has learned in the classroom. "On the one hand," she tells us, "I've learned a lot about Korean culture and language, but [the overall experience] provides a framework for learning more about myself, and what it means to be an American."

Wiest hopes her year abroad and the friends and contacts she makes in Korea will ultimately lay the groundwork for her career. "I hope to tie my career to Korea in the future," she says, "whether it be working for a Korean company looking to expand in the U.S., or a U.S. company in Korea."

FISHER WINS ELECTROCHEMICAL SOCIETY POSTER, TRAVEL AWARDS

ChBE graduate student **Aaron Fisher**, advised by Fischell Department of Bioengineering professor **Peter Kofinas**, received a travel award from the Electrochemical Society's (ECS) Battery Division. The award helped fund Fisher's trip to the 2012 Pacific Rim Meeting on

Electrochemical and Solid-State Science (ECS/PRiME) in Honolulu, Hawaii, in October, where he presented his work on block copolymer battery electrolytes. The prize also included a one-year student membership in the society.



LISA WIEST (FRONT ROW CENTER) WITH MEMBERS OF PROFESSOR IL MOON'S RESEARCH GROUP AT YONSEI UNIVERSITY, SOUTH KOREA.



Fisher won complimentary registration for the conference at the University of Maryland Student Chapter of the ECS's first annual poster contest, where he took first place for a presentation titled "Lithiated Block Copolymer Electrolytes with Ionic Liquids for Batteries."

WU: CATALYSIS CLUB POSTER AWARD



YIQING WU

ChBE graduate student **Yiqing Wu**, advised by ChBE assistant professor **Dongxia Liu**, was one of four first-place winners in the Catalysis Club of Philadelphia's annual Student

Poster Contest, held in October 2012. In addition to the prize, Wu was invited to deliver a presentation at one of the club's monthly meetings.

Wu's poster, "Catalytic Characterization of Hierarchical Meso-/microporous MFI and MWW Zeolites," describes novel lamellar structured zeolite catalyst materials for reaction engineering that could be used to manufacture new or improved industrial chemicals and clean fuels.

The catalysts Wu studies exhibit a high reaction rate and controlled selectivity, allowing them to produce products with greater purity and less waste. If the cost of synthesizing these new catalysts can be reduced, the cost of the high-quality products created with them will be as well.

"The hierarchical MFI and MWW zeolites with unit cell thick crystallite size were synthesized and their catalytic ability was studied by using probe reactions such as dehydration of ethanol and alkylation of benzyl alcohol with aromatic solvents," Wu explains. "The intrinsic catalytic behavior of hierarchical lamellar zeolites is comparable to their microporous counterparts; while in diffusion constrained reactions, hierarchical lamellar zeolites can successfully mitigate diffusion limitations because of the facile mass transport in the novel unit cell thick zeolite crystallites."

WACHSMAN: FUEL CELL SEMINAR & ENERGY EXPOSITION AWARD



ERIC WACHSMAN

University of Maryland Energy Research Center (UMERC) director Professor **Eric Wachsman** (Departments of Materials Science & Engineering and Chemical & Biomolecular Engineering) received the 2012 Fuel Cell Seminar & Energy Exposition (FCS&E) Award. Wachsman and a fellow honoree were recognized at the opening plenary session of the event, held November 6 in Uncasville, Conn.

According to the FCS&E, the awards are given annually "to those who have demonstrated significant leadership in promoting the overall advancement of fuel cell technology," recognizing "both the scope and impact of [the recipients'] research accomplishments and [their] promotion of partnerships that advance research and development and commercialization of fuel cells."

Wachsman is a recognized leader in the development and championing of solid oxide fuel cells (SOFCs) for stationary and automotive power generation.

CHOI APPOINTED TO U.S./KOREA ADVISORY COMMITTEES

ChBE professor **Kyu Yong Choi** has been elected to serve on two prominent international committees focused on fostering research and education partnerships between the United States and Korea.

In December 2012, Choi received a two-year appointment to the Global R&D Advisory Committee of Korea from Korean Ministry of Knowledge and Economy (MKE) leader **Suk Woo Hong**. The committee's mission is to advise the MKE—Korea's equivalent of the U.S.'s Departments of Energy and Commerce—on how best to promote cooperation between the two countries in the area of commercializing intellectual properties, particularly those developed at universities. The



KYU YONG CHOI

committee is expected to propose strategies that use these partnerships to create jobs and programs designed to boost both countries' economic development. Choi says the committee also plans to identify and invite experts in major areas of interest—including energy, IT, and nano- and biomedical technology—to attend joint technical workshops in Korea.

Choi was also elected to the Executive Committee of the Korea-U.S. Science Cooperation Center (KUSCO), which fosters scientific and engineering research and education exchanges between the United States and South Korea. KUSCO is supported by the Korea Research Foundation, the counterpart to the U.S.'s National Science Foundation.

Choi, an elected Permanent Member of the Korea Academy of Science and Technology, is a longtime advocate of scientific collaboration between the two countries, and often encourages students to learn new languages and to study engineering abroad. Recently, he helped ChBE rising junior and group member **Lisa Wiest** secure a Boren Scholarship, which is supporting her study of Korean during the 2012-2013 academic year at Yonsei University in Seoul, South Korea (see p. 8).

"I am happy to help link leading-edge scientific and engineering outcomes with commercialization potential to industries in both Korea and the U.S.," he says of his involvement.

CHOI, BURKA TO REPRESENT U.S. IN WORLD CONGRESS OF CHEMICAL ENGINEERING

ChBE professor **Kyu Yong Choi** and ChBE visiting professor Dr. **Maria Burka** (National Science Foundation and past president, American Institute of Chemical Engineers [AIChE]) will represent the United States on the International Advisory Committee of the 9th World Congress of Chemical Engineering (WCCE). WCCE, the largest international conference on chemical engineering, will be held in Seoul, Korea from Aug. 18-23, 2013.

The Congress draws participants from countries around the world, including the Americas, Asia, Europe, the Middle East, and Oceania. Activities and presentations will reflect the theme "Chemical Engineering: Key to the Future" by emphasizing chemical engineering's role in areas including sustainability, energy, biotechnology, and information technology. Guests will also discuss current trends in and issues affecting chemical engineering in academia and industry.

The Congress' International Advisory Committee is responsible for building a high quality technical program designed to encourage networking, presentation of state-of-the-art research, the exchange of ideas, and new collaborations.

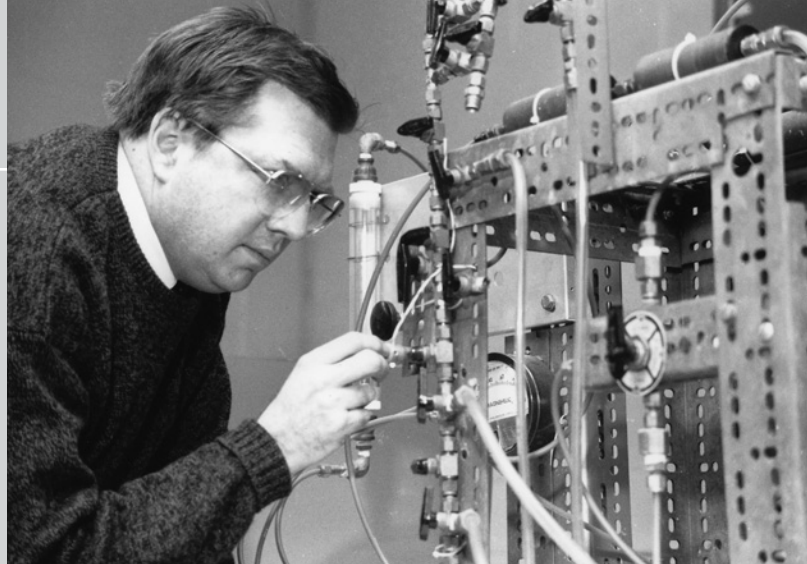
In addition to his duties on the committee, Choi will be chairing sessions on advanced applications in chemical reaction engineering. He says he looks forward to using the professional connections he has built over the past 28 years of his career to make the conference a success and great value for everyone attending.

Choi and Burka will be joined on the committee by fellow U.S. representatives Dr. **Phillip Westmoreland** (North Carolina State University and 2013 AIChE President) and Professor **Arvind Varma** (Purdue).

To learn more about the WCCE, visit www.wcce9.org.

IN MEMORIAM: PROFESSOR EMERITUS JAMES GENTRY

The Department of Chemical and Biomolecular Engineering is sad to report the passing of Professor Emeritus **James W. Gentry**, 72, in his home state of Oklahoma in late October, 2012. Gentry, who

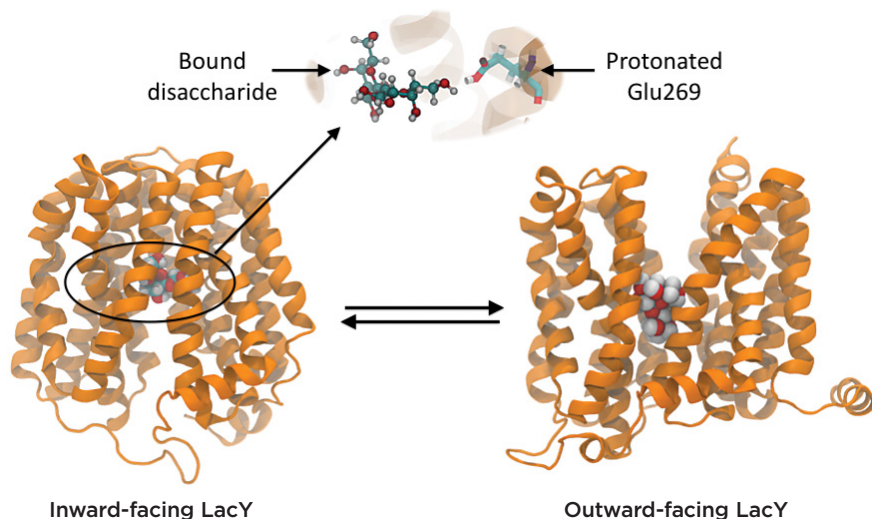


specialized in aerosol mechanics, served on the faculty for 33 years.

The department sent the following letter to Gentry's family and friends for inclusion in his memorial service:

"On behalf of the University of Maryland community we wish to express our sadness at the passing of Professor James W. Gentry... He will long be remembered in his professional community for his brilliant scholarship, working at the interface between applied math, physics, and chemical engineering in the then emerging field of aerosol science and technology. His contributions to aerosol science were broad but were especially significant in the areas of aerosol electrophysics and particle size distribution dynamics. His fundamental work led to improved understanding of processes important for

NSF CAREER AWARD, continued from back cover



(SATs) interact with cell membranes. In most cases, only one conformational state is known for each SAT, but their transport cycles require several conformations in order to move their molecular cargo. The objective of the research is to investigate the transport mechanisms and multiple conformational changes of several SATs through the use of a new simulation method called "implicit-explicit membrane simulation."

"We've extended an existing technique developed at the National Institutes of Health

◀ THE RESULT OF THE KLAUDA GROUP'S NEW ENHANCED SIMULATION TECHNIQUE TO PROBE STRUCTURAL CHANGES IN THE LACTOSE TRANSPORTER OF *E. COLI* FROM ITS KNOWN STRUCTURE (INWARD-FACING) TO A PREVIOUSLY UNKNOWN STRUCTURE (OUTWARD-FACING). PROTONATION OF RESIDUE GLU269 WAS FOUND TO BE IMPORTANT IN TRANSITIONING FROM THE INWARD- TO OUTWARD-FACING STATE.

reducing air pollution, improving powder manufacturing, and improving sampling of aerosols relevant to occupational health. In addition to his scientific contributions, he was also one of the historians of the discipline, and he could trace the evolution of ideas and the people behind them back as far as the 1800s.

“On campus, Professor Gentry will be remembered as a teacher, mentor, scientist and colleague. He trained numerous successful scientists and engineers, who are working around the world in industry, laboratories and academia. In addition, he mentored many junior faculty [members], both in and outside of his scholarly field of research. He took awards, of which he won many, very seriously; and was proactive in nominating and securing recognition for many deserving colleagues and students...

“Professor Gentry was an avid collector of books, and upon his return to Oklahoma, he helped to establish a library in the department of his technical book collection that also includes books related to his other pursuits. We possibly are now the only

engineering department in the U.S. with a library containing books on Ellsworth Kelly, Meissener porcelain, pulsed neutron research, and the French Revolution, and that’s just from a single shelf.

“Professor Gentry was the first to jump to the chalkboard to walk a curious student through some elaborate mathematics, the first to suggest a lunch at Seven Seas, the nearby Chinese restaurant, or the first to talk about an art exhibit he had seen during his most recent trip abroad...He was diligent about staying in touch with us through e-mail, phone [calls] and in person at scientific conferences, and we appreciated his active interests in the goings on in our department. We have missed him greatly since he returned to his native Oklahoma several years ago; and more so now.”

SENGERS HONORED

Distinguished University Professor Emeritus **Jan V. Sengers** (joint, ChBE and Institute for Physical Science and Technology [IPST]) was a guest of honor at the 108th Statistical Mechanics Conference held at Rutgers, the State University of New Jersey. Sengers was recognized for his “seminal contributions, both experimental and theoretical, to our understanding of fluctuations nonequilibrium fluids” at the event’s gala dinner on December 17. Sengers’ longtime colleague, Professor **Mikhail Anisimov** (ChBE/IPST) also attended the conference, where he delivered a talk on entropy-driven liquid-liquid transitions in pure substances.



PROFESSOR **JAN SENGERS** (RIGHT) WAS ONE OF THREE PROFESSORS HONORED AT THE 108TH STATISTICAL MECHANICS CONFERENCE HELD AT RUTGERS, THE STATE UNIVERSITY OF NEW JERSEY. WITH SENGERS ARE FELLOW HONOREES **JOHN REPPY** (CORNELL, CENTER) AND **HARRY SWINNEY** (UNIVERSITY OF TEXAS, LEFT).

called self-guided Langevin dynamics, or SGLD, that enhances motions based on a random guiding force,” explains Klauda. “Although this has been used in peptide [short amino acid sequences] folding studies, we were the first to successfully extend it to significant changes in a large transmembrane protein. The novelty of our approach is that SGLD is only used to obtain conformations that are placed in an all-atom explicit membrane model of *E. coli*. These are then simulated with molecular dynamics to obtain equilibrated structures that closely match the environment in the cell.

“The exciting part of research,” he adds, “is that we will be able to provide a clearer

picture of membrane protein transport cycles that have eluded scientists for nearly all SAT proteins. Obtaining high-resolution crystal structures of SAT proteins is extremely tricky. Our new discoveries will certainly complement those in traditional protein structural determination.”

In addition to contributing to our fundamental understanding of protein transport in the cell membranes of mammals, plants and single-celled organisms, Klauda’s work may also shed light on problems such as why and how drug-resistant cells expel antibiotics.

Klauda feels the University of Maryland has been an excellent place to launch his

academic career. “The computational support provided by the Office of Information Technology’s Deepthought High Performance Computing Cluster has allowed my students to focus on science and provides ample resources for our computationally demanding studies,” he says. “UMD’s closeness to national labs like the NIH and NIST has enhanced our ability to collaborate with their experimentalists and theoreticians.”

For More Information:

Pendse, P. Y., Brooks, B. R., and Klauda, J. B. (2010). Probing the Periplasmic-Open State of Lactose Permease in Response to Sugar Binding and Proton Translocation. JMB 404, 506:521 <http://tinyurl.com/2b9k6dw>



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ABOUT THE COVER IMAGE

THE BLUE IMAGE USED ON THE COVERS SHOWS A MEMBRANE TRANSPORT PROTEIN, LACTOSE PERMEASE (PROTEIN HELICES REPRESENTED IN SHAPE OF RODS), EMBEDDED IN A MODEL *E. COLI* MEMBRANE, DEVELOPED IN THE RESEARCH GROUP OF CHBE ASSISTANT PROFESSOR JEFFERY KLAUDA. THE SPHERES ABOVE AND BELOW OF THE MEMBRANE REPRESENT WATER MOLECULES. KLAUDA'S GROUP HAS DEVELOPED A HYBRID SIMULATION METHOD TO STUDY STRUCTURAL CHANGES IN MEMBRANE TRANSPORT PROTEINS, FOR WHICH KLAUDA RECEIVED A NATIONAL SCIENCE FOUNDATION FACULTY EARLY CAREER DEVELOPMENT (NSF CAREER) AWARD. FOR MORE INFORMATION, SEE THE STORY BELOW.

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NSF CAREER Award for Advanced Simulations of Protein Transport in Cell Membranes



JEFFERY KLAUDA

A proposal to use the first all-atom technique to predict, in an unbiased manner, the structural transitions that occur in proteins that transport molecules through cell membranes has earned Department of Chemical and Biomolecular Engineering assistant professor

Jeffery Klauda a 5 year, \$688,313 National Science Foundation Faculty Early Career Development (NSF CAREER) Award. The NSF CAREER program supports the career development of outstanding junior faculty who most effectively integrate research and education within the goals and missions of their programs, departments, and schools.

Klauda studies the ways in which cell membrane transport proteins act as gatekeepers, allowing helpful molecules in, and expelling or denying entry to harmful ones. They accomplish this by reconfiguring their conformations, or structures: they are either open to the outside or to the inside

of the cell. After collecting a molecule, they “swing shut” on that end, “swing open” on the other, and expel it on the opposite side, like a revolving door designed for a single person. Klauda's research group has been developing a novel computer simulation technique that visualizes, explains and predicts the proteins' behaviors.

Klauda's award-winning proposal, “Secondary Active Membrane Transporters: Determining Protein Structure and Transport Mechanism with a New Hybrid Simulation,” outlines his plan to investigate how a class of proteins called secondary active transporters

continues on page 10