Notre Dame Science

The magazine of the College of Science at the University of Notre Dame

Spring 2017

DISCOVER

Frontiers in science

MARY GALVIN
William K. Warren Foundation Dean
of the College of Science

In this issue of Notre Dame Science, we focus on discovery across all scientific disciplines. You will read about McCourtney Hall, our new, interdisciplinary, research facility fostering scientific collaboration between scientists and engineers. Notre Dame has been home to world-renowned mosquito research since the mid-1950s, and we continue to lead new research, including focus on solving the Zika virus epidemic. Among other topics, you will learn: astrophysicists in our galactic archaeology group led discoveries about how the Milky Way galaxy was formed, faculty in chemistry and biochemistry have discovered two new classes of antibiotics with the potential to treat the superbug MRSA, applied and computational mathematicians are solving big problems by analyzing big data, and faculty and students have developed inexpensive and easy-to-use methods to identify counterfeit medications.

We are proud of Notre Dame Science faculty and students. Science researchers have received 24 patents in the past five years, many for discoveries with potential to treat illnesses. In 2016, eight graduate students from the College of Science were awarded NSF Graduate Research Fellowships and another seven received honorable mentions.

The College of Science strengthens the pursuit of scientific discovery among our students, and faculty. Our undergraduates discover their passion for a field of research, our graduate students and researchers discover new ways to solve scientific problems, and our faculty guide these pursuits while developing an exceptional new generation of inspired scientists. Discovery fuels our passion for this work. I think you'll agree that Notre Dame is the perfect place to discover what's possible.

Sincerely,

Mary E. Galvin

MARY E. GALVIN, PH.D.
William K. Warren Foundation Dean of the College of Science
Professor of Chemistry

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Front cover photo: This magnified photo shows an *Aedes aegypti* mosquito larva at the fourth instar stage of development. Actual size is approximately eight millimeters. Photo credit: Matt Cashore, Univeristy of Notre Dame

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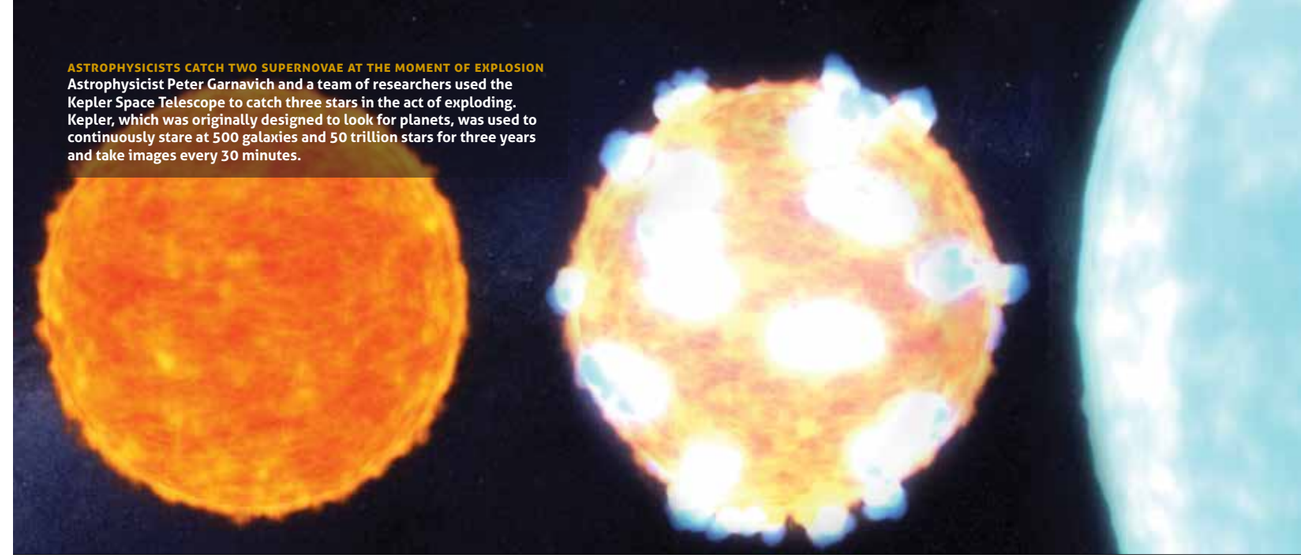

ASTROPHYSICISTS CATCH TWO SUPERNOVAE AT THE MOMENT OF EXPLOSION
Astrophysicist Peter Garnavich and a team of researchers used the Kepler Space Telescope to catch three stars in the act of exploding. Kepler, which was originally designed to look for planets, was used to continuously stare at 500 galaxies and 50 trillion stars for three years and take images every 30 minutes.

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UNIVERSITY OF NOTRE DAME
College of Science

McCourtney Hall fosters collaboration, interdisciplinary research, and discovery

By Tammi Freehling

MCCOURTNEY HALL, A NEW RESEARCH facility, opened in fall 2016 on the northeast side of campus. The 220,000-square-foot building dedicated to research in the molecular sciences and engineering is designed to promote interdisciplinary research and enhance collaborations. Researchers from the College of Science and the College of Engineering are intentionally grouped together by interest area into "neighborhood" labs. Social common areas foster natural conversations, which can advance problem solving across different teams.

"McCourtney Hall is expected to lead to more collaborative and stronger interdisciplinary research," noted Brian Baker, Rev. John A. Zahm Professor and chair of the Department of Chemistry and Biochemistry. "Collaborative science is the way of the future. You can't do anything nowadays without working with somebody else, usually in a very different discipline."

As the first building in the planned East Campus Research Complex, McCourtney Hall, "creates a great opportunity for the research programs in science and engineering at Notre Dame," said Robert Bernhard, vice president for research at Notre Dame. "The building is designed as a collaborative and adaptive space to encourage cross-disciplinary research interaction along the entire continuum of basic and applied research. We expect the building to be a game-changer for science and engineering research at Notre Dame." More than 200 people, including nearly 40 faculty members, work in McCourtney Hall. And some 40,000 square feet of laboratory space is intentionally unoccupied to accommodate future new faculty hires.

Research in McCourtney Hall is focused on three key areas: analytical sciences and engineering, chemical and biomolecular engineering, and drug discovery. From brain injuries to clean water, cancer treatment to sustainable energy and climate change, research within McCourtney Hall is conducted to discover new technologies in the face of the world's grand challenges and to advance Notre Dame's mission to be a powerful force for doing good in the world.

McCourtney Hall was underwritten with a $35 million gift from alumnus Ted H. McCourtney and his wife, Tracy. Thomas J. Crotty Jr. and his wife, Shari, also provided a $10 million gift in support of the building. ■

Feature

Notre Dame fights Zika epidemic

By Gene Stowe

WHEN THE WORLD HEALTH ORGANIZATION declared the Zika virus epidemic in the Americas as a Public Health Emergency of International Concern in early 2016, Notre Dame scientists were positioned to lead the fight. Building on the world-leading mosquito research established by George Craig decades ago to combat diseases such as malaria and dengue fever, as well as new tools to predict the spread of infections, College of Science faculty members working in the Eck Institute for Global Health are opening new lines of attack aimed at the vectors that carry the virus. Because the work is not limited to Zika specifically, it offers weapons against a variety of other mosquito-borne illnesses.

A paper by Assistant Professor **Alex Perkins** and others, published in July 2016 in *Nature Microbiology*, provides a rigorous approach to rapidly predicting the spread of the epidemic by focusing on local conditions rather than aggregate data from large countries like Brazil or Mexico. Companies that are developing Zika vaccines are using the information to select areas where they will conduct trials of their own vaccines. The researchers concluded that some 1.65 million childbearing women could be infected in the first wave of the epidemic, far fewer than earlier estimates of up to 5.42 million women yet still indicating that tens of thousands of pregnancies could be at risk. Overall, more than 90 million people could be infected in the first wave of the epidemic.

Data about individual Zika cases is scarce because most who are infected show no symptoms, many more do not seek treatment, and limited diagnostic tests often cannot distinguish Zika from other viruses. However, earlier research on dengue and chikungunya viruses yielded vital information about the ecology of the disease and the role of the mosquitoes that transmit it. Perkins said the mathematical model considers such factors as density of the Zika-bearing *Aedes aegypti*, prevailing temperatures, and the availability or lack of air conditioning that affects the risk of mosquito bites in a particular locale, in order to gauge what portion of the population could be at risk.

Epidemics burn themselves out in different geographic areas as more people develop immunity over time. In this case, useful location-specific data available online from Colombia helped reveal patterns that are masked by the aggregate data in larger countries where the infections can vary widely from place to place. The work was funded by a National Science Foundation grant for Rapid Response Research (RAPID).

Under another grant from the military's Defense Advanced Research Projects Agency (DARPA), Perkins is conducting research on chikungunya, another mosquito-borne virus that appeared in the Americas in late 2013. "Chikungunya and Zika have popped up and become major issues since I came to Notre Dame," said Perkins, who has conducted extensive research on dengue and malaria. The predictive model developed for Zika can be applied to all of those diseases.

The paper, "Model-based projections of Zika virus infections in childbearing women in the Americas" by T. Alex Perkins, Amir S. Siraj, Corrine W. Ruktanonchai, Moritz U. G. Kraemer, and Andrew J. Tatem, is available at nature.com/articles/nmicrobiol2016126.

Associate Professor **Mary Ann McDowell**, who came to Notre Dame in 2001 and started focusing on mosquitoes five years ago because of the University's strong position in the field, investigates ways to develop novel insecticides. The aim is to kill mosquitoes, which can become resistant to conventional insecticides, and help in the fight against several major diseases at once, including Zika and others that might arise after the current epidemic subsides.

One project with funding from the U.S. Department of Defense takes a two-pronged approach—understanding mosquito behavior and identifying chemicals that will kill them. By screening chemical libraries, McDowell has identified compounds that interfere with certain receptors in the mosquito's body, killing both larvae and adults without being toxic to humans. Her lab is seeking to improve those chemicals. She is collaborating with Assistant Professor Zain Syed, who studies how the chemicals affect mosquito behavior, and Bruce Melancon, a research assistant professor and managing director of the Chemical Synthesis & Drug Discovery Facility, which synthesizes chemistries designed to be more stable and effective within the mosquito.

Assistant Professor **Zain Syed** focuses primarily on the role of olfaction, the sense of smell, in mosquito behavior, particularly the way the insects are attracted to or repelled by human odors. He collects those odors, gauges the response they elicit in mosquitoes, and attempts to identify the chemical constituents responsible. Knowing the chemicals that attract mosquitoes can provide bait for traps to destroy them; knowing the chemicals that repel mosquitoes can provide applications that prevent bites. Mosquitoes are less likely to develop resistance to such repellents because they are occasionally on the skin, bed nets, or other areas, rather than in a constant way, as would be the case with insecticides that would drive natural selection against mosquitoes.

The leading vectors that carry Zika are *Aedes albopictus* and *Aedes aegypti*. In his earlier research, Syed focused on the *Culex* mosquito, which routinely feeds on birds until bird populations migrate, and then begins to feed on humans. He identified a specific chemical, nonanal, that birds and humans have in common,

Assistant Professor ZAIN SYED works in his lab with a student. Research in the lab involves the sense of smell in mosquito behavior.

ALEX PERKINS

MARY ANN MCDOWELL

ZAIN SYED

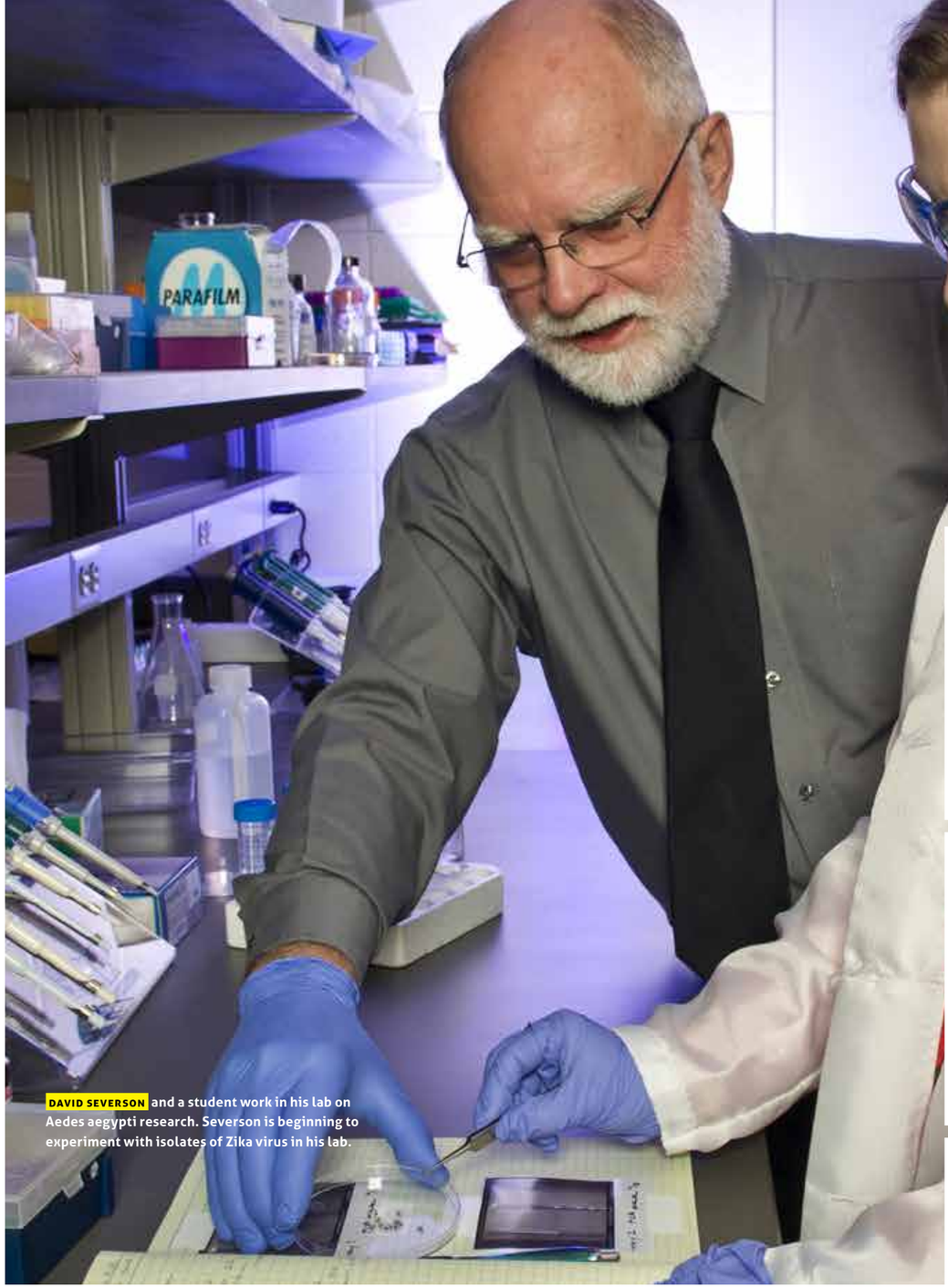
and it turned out to be highly attractive to mosquitoes. He is conducting similar research now on *Aedes*.

Also in Syed's laboratory, a student is on a mission to study the microbiome in the gut of *Aedes* samples collected in regions infected by Zika, in order to see how the mosquito protects itself from pathogens in the blood it consumes. The microbiome influences what the organism smells and how. A visiting researcher from Brazil demonstrated that removing the gut bacteria compromises the mosquito's ability to function.

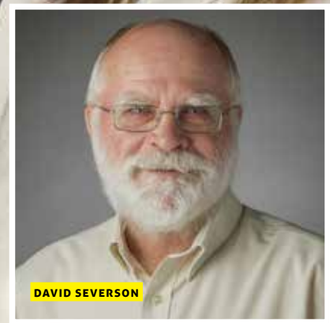
Professor **David Severson**, who has studied *Aedes aegypti* since he came to Notre Dame 20 years ago, said his research has direct application to Zika, although he is only beginning to experiment with isolates of the virus in his laboratory. Severson has focused on studies of how the mosquito immune system responds to infection by dengue virus. After feeding an infected artificial blood meal to the mosquito, he extracts its RNA and considers each gene in the genome to detect whether the dengue virus is expressed. Pathways related to innate immunity in insects are nearly identical to those in humans. Results from these studies may lead to new disease prevention strategies.

Severson, who has studied various viruses in different mosquito populations, expects close parallels in the innate immune response with Zika. Apart from the added risk of microcephaly, he said Zika poses less risk to humans worldwide than several other mosquito-borne viruses. Dengue, for example, comes in four varieties, or serotypes, that can each infect a person even when they have gained an immunity to the other varieties. Zika, first identified in 1949, had been a relatively benign virus until the recent outbreak in the Americas, and the cause of the virus is still unknown.

Research Associate Professors **Nicole Achee** and **John Grieco**, associate director of the Eck Institute, collaborate on research that focuses on helping resource-limited countries in Central and South America detect such viruses as Zika, dengue, and chikungunya. Their work includes training lab technicians and local vector control officers; testing samples from both humans and mosquitoes to pinpoint the location of Zika and other viruses; helping governments provide public education about the diseases; and developing mosquito control tools such as traps, repellents, and insecticides. The researchers help local partners evaluate control measures to determine effectiveness. Their ultimate research goal is to accelerate the fight against Zika and establish ongoing community health benefits against other diseases carried by *Aedes* mosquitoes. ■



DAVID SEVERSON and a student work in his lab on Aedes aegypti research. Severson is beginning to experiment with isolates of Zika virus in his lab.



DAVID SEVERSON

NICOLE ACHEE

JOHN GRIECO

ALEX PERKINS and graduate student Amir Siraj work on research to estimate and forecast Zika transmission.

Using mathematical models to strategically fight the Zika virus

By Gene Stowe

Alex Perkins, Eck Family Assistant Professor of Biological Sciences, received a rapid response grant (RAPID) from the National Science Foundation's (NSF) Division of Environmental Biology's Ecology and Evolution of Infectious Diseases Program for his research proposal that focuses on enabling estimation and forecasting of Zika virus transmission. NSF created these RAPID awards to specifically understand the rate of spread, the number of infected people, and the likely persistence of Zika as a public health threat, ultimately to help prepare for the next outbreak.

Results from the project will benefit Zika public health emergency response, as researchers will have tools in place to share quality data and forecasts both during the study and after the project concludes. This will be a valuable asset for policymakers as they continue to make decisions surrounding this virus.

"This grant will allow us to contribute a number of data and modeling products to the academic and public health communities, including improved estimates of spatial and temporal variation in mosquito densities, improved estimates of spatial variation in birth rates, and mathematical models that better account for unique aspects of Zika's epidemiology," Perkins said.

Zika is primarily transmitted to humans through the bite of an infected Aedes aegypti mosquito, a species that the University of Notre Dame has nearly 60 years of experience studying. Perkins' research will provide estimates of Aedes aegypti mosquito density across the Americas, as well as updated human population data as it applies to predictions of Zika-infected microcephaly.

Perkins is associated with the Eck Institute for Global Health, a University-wide enterprise that recognizes health as a fundamental human right and endeavors to promote research, training, and service to advance health standards for all people, especially those in low- and middle-income countries who are disproportionately impacted by preventable diseases.

Picture this: Discovering how our galaxy formed

By Brian Wallheimer

ASTRONOMERS AND ASTROPHYSICISTS curious about how our own Milky Way Galaxy formed have the clearest picture yet, based on the work of Notre Dame's Timothy Beers and his Galactic Archaeology Group.

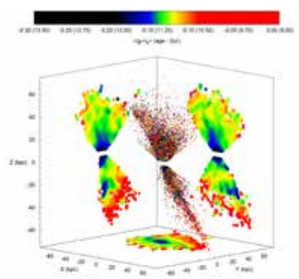
The group first put together a chronographic (age) map that shows how the Milky Way formed by merging and accretion of small mini-halos containing stars and gas. They also found that the oldest of the Milky Way's stars are at the center of the galaxy, and that younger stars and galaxies merged with the Milky Way, drawn in by gravity over billions of years. The map was built using spectroscopic data from the Sloan Digital Sky Survey, which gave the researchers the opportunity to estimate ages for 4,700 horizontal-branch (BHB) stars, blue stars that burn helium in their cores.

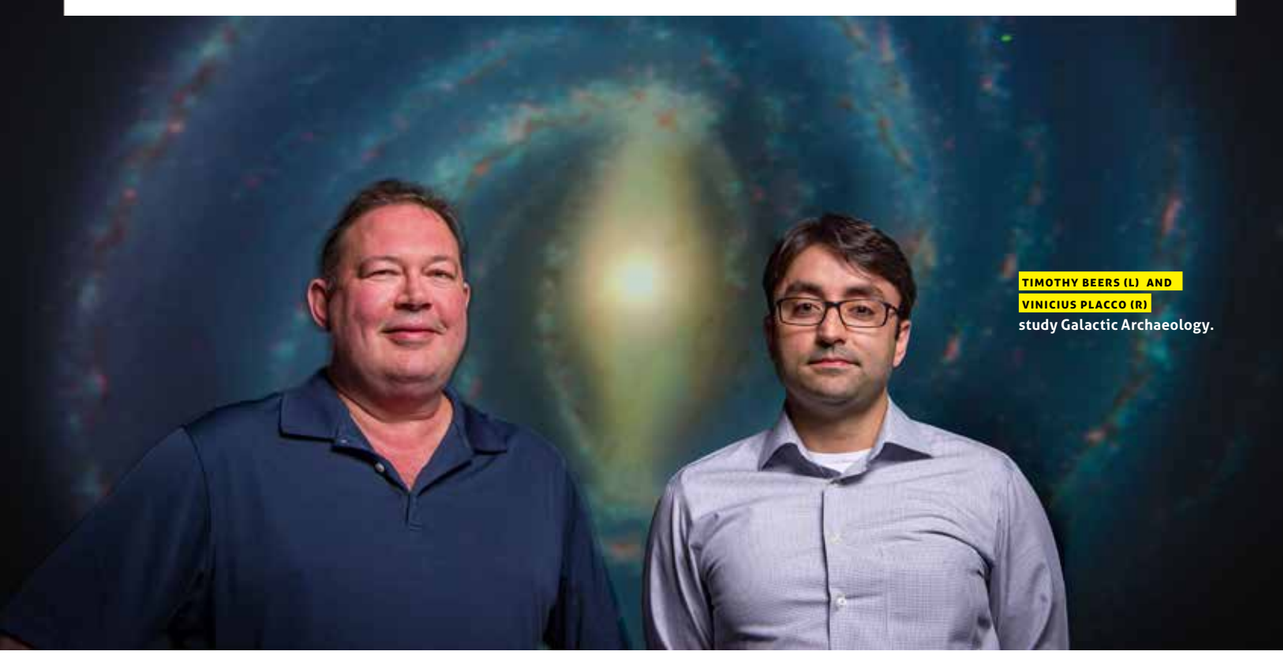
The map also confirmed a method for aging stars that Beers began developing 25 years ago. His group showed that the ages of these BHB stars can be determined by color alone.

With this method, the group used photometry to age-date more than 130,000 stars and constructed a far more detailed map that helped identify the location of more galactic structures. "The colors when the stars are at that stage of their evolution-are directly related to the amount of time that star has been alive, so we can estimate the age," Beers said. "We can now actually visualize how our galaxy was built up and inspect the stellar debris from some of the other small galaxies being destroyed by their interaction with ours during its assembly."

Vinicius Placco, research assistant professor of astrophysics, said the first map was built using a minimum of three stars per pixel, which meant it had to be "folded over" (combining the Southern Galactic Hemisphere with the Northern Galactic Hemisphere) to include enough data points to give a clear picture. The new map has at least 10 stars per pixel and can be expanded fully to get a more detailed picture of the galaxy's progression.

"In the first map we were able to identify some of these structures, but we weren't able to tell where these structures really were," Placco said. "In the new map, you can see all of those structures. It tells us how complex the assembly of the galaxy was. We are now able to test new predictions and use the map to test new models of the chemical evolution of the galaxy." ■





TIMOTHY BEERS (L) AND VINICIUS PLACCO (R) study Galactic Archaeology.

Antibiotic discoveries combat superbug MRSA

By Brian Wallheimer

PATIENTS DEALING WITH MRSA AND OTHER antibiotic-resistant bacteria currently have just a few options for treatment. Soon, they may have two more.

Department of Chemistry and Biochemistry faculty Shahriar Mobashery, the Navari Family Professor in Life Sciences, and Research Professor Mayland Chang have discovered two new classes of antibiotics that show promise for treating methicillin-resistant *Staphylococcus aureus*, or MRSA. The hard-to-kill bacterium is a so-called superbug because it can rapidly develop resistance to antibiotics, giving medical professionals few options for helping patients.

MRSA is more common in hospitals but also has been spreading in other places where large populations gather, including prisons, schools, and locker rooms. In 2011, MRSA resulted in more than 80,000 infections and 11,000 deaths, according to the Centers for Disease Control and Prevention.

Combing through a database of more than 1.2 million known compounds, Mobashery and Chang identified 20 that had the potential to kill MRSA bacteria. From there, they narrowed the list to two—quinazolinones and oxadiazoles.

"These antibiotic classes were discovered by searching for compounds that had the ability to interfere with the biosynthesis of bacterial cell wall," Mobashery said.

The discoveries are especially important because they are new classes of antibiotics, rather than new antibiotics in already-known classes. Discovering a new form of penicillin might be helpful, but MRSA and other bacteria quickly develop resistance because of their similarities to other penicillin drugs.

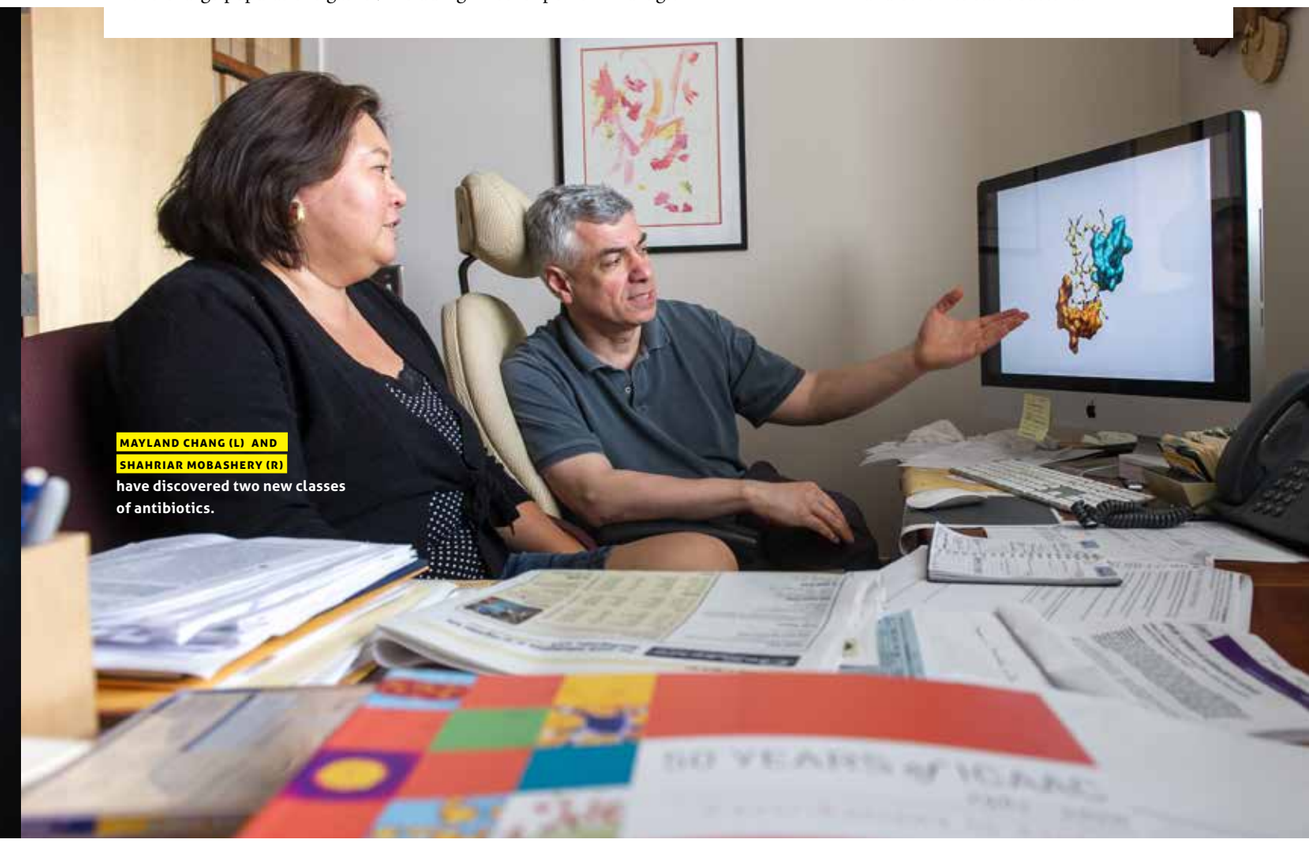
New classes, which the bacteria have not encountered, provide opportunities in treatment of infections that did not exist previously.

Mobashery and Chang have identified a variant of an oxadiazole that can be taken orally, which is desirable for any drug. The compounds are efficacious in animal models of infection, which translate well to patients.

"It can rescue mice from the infection and compares well, or is superior to linezolid, the current gold standard oral anti-MRSA agent," Chang said.

Zolex Therapeutics has licensed both classes of drugs and intends to bring them to market.

"We're excited to have discovered these new classes of antibiotics," Mobashery said. "Having these tools available may have a significant impact on the health of patients who find themselves dealing with MRSA and other resistant bacteria." ■



MAYLAND CHANG (L) AND SHAHRIAR MOBASHERY (R) have discovered two new classes of antibiotics.

Digging into big data to solve big problems

By Brian Wallheimer

ADVANCES IN TECHNOLOGY HAVE PROVIDED scientists with vast amounts of data that could be key to advances in health care, technology, and many other fields. But first, people must learn how to sort, organize, and pick through that so-called big data to make use of it.

Notre Dame's big data scientists are doing just that, from creating valid and efficient statistical models to crunch numbers to applying those models to advance cancer technology.

Lizhen Lin and Jun Li, both assistant professors in the Department of Applied and Computational Mathematics and Statistics, develop models to cut through the noise of big data and find useful information.

"We are living in this modern time with big data—it's everywhere. In all kinds of different fields, you have a lot of data, and the data are often, in addition, complex and high-dimensional" Lin said. "We need to develop statistical models to understand that data better, to make better decisions."

Lin, in her research funded by the National Science Foundation Big Data program, develops statistical models that can extract lower-dimensional structure in high-dimensional space. These models can be used to organize and classify noisy information. The same model can be applied to other fields, including detecting genes for certain types of cancer.

Li develops modern statistical machine learning methods that can take thousands of variables into account.

"The data is very noisy, and there may be 10,000 Xs, and you need to use them to predict a single Y," Li said. "We not only want to avoid overlearning and accurately predict Y, but we also want to know which Xs are important to the prediction of Y. This mission was almost impossible but now is totally manageable by using tools such as Lasso and its variants." Lasso (least absolute shrinkage and selection operator) is a process for estimating relationships among variables in order to enhance prediction accuracy and interpretability of the statistical model it produces.

Steven Buechler, professor of applied and computational mathematics and statistics, uses big data to pinpoint the molecular markers associated with breast cancer. He is able to identify tumors likely to need alternatives to traditional chemotherapy regimens, as well as tumors that may not need chemotherapy at all. But that involves working through the complex interactions of hundreds, even thousands, of molecules.

"We're looking for patterns that point to clinically relevant information about the tumor," Buechler said. "This gives us a picture of the state of the tumor, but it's a very complicated picture because you have all these possible molecules to look at. You can't focus your attention on just a few molecules. You have to look at the whole picture."

Fang Liu, Huisking Foundation, Inc. Assistant Professor of Applied and Computational Mathematics and Statistics, is optimistic about the future of big data research at Notre Dame. Several statistician hires will join others in the coming years, adding depth to those involved in the field.

"Notre Dame definitely sees the opportunity to invest in big data research," Liu said. "We're hiring faculty with quantitative skills throughout the University, and that will enhance Notre Dame's research profile and impact on the field of big data." ■

LIZHEN LIN, FANG LIU, STEVEN BUECHLER, AND JUN LI work with big data to tackle problems in a diverse array of fields.

It's in the cards

By Marissa Gebhard

According to the World Health Organization (WHO), nearly half of the world's population is at risk for contracting malaria. Despite a 29 percent reduction in mortality rates since 2010 due to prevention and control measures, nearly 430,000 people died of malaria across the globe in 2015. Ninety-two percent of deaths from malaria occur in Sub-Saharan Africa.

There are many effective anti-malarial medications on the market, including chloroquine, doxycycline, sulfadoxine, and pyrimethamine. Yet among others, but in the developing world, many patients who vitally need these medications are left with no other choice than to purchase a medication that could be substandard or counterfeit. In 2011, 64 percent of anti-malarial medications in Nigeria were fake, according to the WHO, and 70 percent of those medications were imported. Until now, neither pharmacist nor patient had any way to know whether medications were legitimate or counterfeit.

Counterfeit medications—those which deceptively represent their authenticity, effectiveness, or origin—may contain improper quantities of active ingredients or none at all. While inert ingredients simply will not treat the patient's condition, improper dosages or hazardous ingredients have been fatal. According to research conducted by the WHO, more than 120,000 people in Africa die each year from fake anti-malarial drugs that were either substandard or contained no active ingredient.

Marya Lieberman, professor of chemistry and biochemistry, has been working to address the counterfeit drug problem, particularly in the developing world where access to expensive testing equipment is prohibitive. Her lab has developed a simple, cost-effective, paper-based test card that can be used in the field to detect the authenticity of medication. The Paper Analytical Device (PAD) has 12 unique lanes that detect common ingredients in counterfeit medications. While it does not replace high performance liquid chromatography (HPLC), which reveals precise quantities for each ingredient, the PAD does reveal which medications are suspicious and therefore should be avoided.

Since 2010, Lieberman's lab has developed PADs that can identify 60 different falsified medications. Her team of undergraduate and graduate students has tested numerous materials and has produced 15,000 test cards. They have traveled to Kenya and Uganda to collaborate with pharmacists and train local patients in the use of the cards.

> It is estimated that up to 30 percent of drugs sold worldwide are counterfeit and account for the deaths of one million people annually.

Lieberman has created a network of 18 universities that utilize their own HPLC machines to aid in the quantitative chemical analysis of medications from pharmacies in Kenya and other developing countries. In January 2016, she guided her Kenyan partner pharmacy through the process of setting up its own HPLC equipment.

This past May, Lieberman and her colleagues, Toni Barstis, professor of chemistry and physics at Saint Mary's College, and Patrick Flynn, Duda Family Professor of Engineering, received a patent titled, "Analytical devices for detection of low-quality pharmaceuticals" for their unique ability to detect at least two chemical components indicative of a low-quality pharmaceutical product, and the method of use thereof. The University of Notre Dame is now negotiating a licensing agreement with a company that will use the invention to help those in the developing world.

Students have played integral roles in every step of the project. Through the Lieberman lab's partnership with American Model Providing Access to Healthcare (AMPATH), undergraduate and graduate students have traveled to Kenya to set up donated HPLC instrumentation. This past summer, during an undergraduate research training session, students discovered an adulterated sample of amoxicillin from Kenya. They reported their analysis of several packages to the WHO Rapid Alert system, as well as the Kenyan medical regulatory authorities, and the product was quarantined. "In Kenya, amoxicillin is the primary medication used to combat acquired pneumonia," Lieberman said. "So the quality of the amoxicillin really matters."

Through a collaboration with Chemists Without Borders, Lieberman leads the Distributed Pharmaceutical Analysis Lab, a network of 18 universities that utilize their own HPLC instruments to aid in the quantitative chemical analysis of medications from pharmacies in Kenya, Uganda, Tanzania, India, Nepal, and Malawi.

MARYA LIEBERMAN works with Mercy Maina, Ampath pharmacist; Sarah Bliese, Hamline University student; and Phelix Were, Ampath pharmaceutical technologist, on the paper analytical device (PAD) project at the Ampath Centre in Eldoret, Kenya in June 2016.

One of Lieberman's successes lies in her collaborative approach to solving such a complex, international problem. Lieberman has partnered with Christopher Sweet, research assistant professor in the Center for Research Computing, to develop a computer-based analysis of PAD results. Lieberman explained, "Chris has been working on a neural network image analysis program. It uses different layers of processing to help distinguish images." The researchers have started to train the neural network to develop rules, and are continually developing larger training sets.

To increase the reach of the PAD, Sweet and Lieberman have collaborated with Da Wi Shin and Bishoy Ghopal, a team of social entrepreneurs from CUNY who created a card reader app called Veri-PAD. Sweet assisted in the creation of their mobile app, and this past summer Shin and Ghopal began piloting the technology with health centers and pharmacies in Kenya and Lebanon.

This past summer, Lieberman's lab sent 277 unknown samples to the Kenyan pharmacist, and they compared human analysis with the image analysis technologies. "So far, the humans are slightly better than the image analysis, but the image analysis programs will improve," Lieberman said.

"The biggest surprise for me is how little of this has been a technology problem," Lieberman continued. "The problems are legal, and they are policy problems. They're business issues. It's not just the science. There are thousands of papers published on sensors, for example, but most of those [inventions] never make it out of the ivory tower. When we began this project, we didn't want to work on something that only worked in the lab. We wanted to do something that worked in the real world, but that turns out to be really complicated." ■

$23 million award at Notre Dame fights malaria and dengue fever

By Marissa Gebhard and Gene Stowe

UNIVERSITY OF NOTRE DAME BIOLOGISTS Nicole Achee and Neil Lobo are leading a five-year international $23 million research grant from the Bill & Melinda Gates Foundation aimed at demonstrating the effectiveness of a new paradigm in mosquito control—spatial repellency—for preventing the major mosquito-borne diseases malaria and dengue fever. The grant is the second largest in Notre Dame history.

The World Health Organization says 212 million cases of malaria were reported in 2015, a 21 percent increase since 2010, although mortality rates fell nearly 30 percent. Forty percent of the world is at risk for dengue fever, and 390 million people are infected each year. Both the malaria parasite and the dengue virus are transmitted by mosquitoes, but mosquito control efforts such as bed nets and spraying have not solved the problem.

Achee and Lobo, research associate professors in the Department of Biological Sciences and members of the Eck Institute for Global Health, are co-principal investigators in the project titled "Spatial Repellent Products for Control of Vector-borne Diseases." Their team includes researchers and advisers from five countries in South America, Africa, and Asia.

The research measures the benefit of using a spatial repellent product to prevent human infections transmitted by several Anopheles species of mosquitoes. In addition to generating the scientific evidence required to demonstrate the effectiveness of the intervention, the work aims to inform global health policy by working with international, regional, and local public health authorities. Spatial repellents can be deployed alone or in conjunction with other strategies.

"The role for repellency to provide protection to people from arthropod-borne diseases, such as malaria and dengue fever, was first recognized more than 50 years ago; however, spatial repellent products have yet to be fully recommended for inclusion in public health programs," Achee said. "Our team has now been given the opportunity, as well as the responsibility, to advance these products to those populations in most need."

"We have data that show spatial repellents are effective against insecticide resistant populations, which may have the potential to limit the spread or emergence of insecticide resistance—one of the many challenges faced by public health officials today," Lobo said. "Residual transmission is also a significant global concern. When combined with other tools we expect they will prove to be even more effective."

"This grant is exactly the kind of research Notre Dame excels in," said David Severson, director of the Eck Institute for Global Health. "We have a long tradition of leading the world in insect-transmitted infectious disease research with networks all over the globe." ■

NICOLE ACHEE

NEIL LOBO

Pavel Mnev
Assistant Professor, Mathematics
Research: Applications of topology to physics

Andrew Putman
Professor, Mathematics
Research: Geometry and topology and their interactions with group theory

Christopher Schommer-Pries
Assistant Professor, Mathematics
Research: Applications of topology, and especially higher category theory to quantum field theory

Topology hires keeping Math "in the thick of things"

By Brian Wallheimer

TOPOLOGY IS A LARGE AND ACTIVE AREA OF MATH THAT CONCERNS properties of shapes that are robust in the sense that stretching and bending do not alter them. Ask a group of first-graders to draw their teacher and the results will vary wildly, but nearly all will involve four limbs and a head. It is these broad features of geometric objects that topologists aim to isolate and understand, though often in far less visually accessible situations with many dimensions and various other complications. Like many modern areas of math, the early development of topology was a mostly theoretical endeavor, undertaken by mathematicians driven by curiosity and aesthetic concerns. As happens remarkably often with such things, topology then found applications to physics (for instance, the most recent Nobel Prize-winning work in physics), biology (the structure of DNA), and statistics (finding trends in large, high-dimensional data sets).

For decades, a core of seasoned mathematicians has built and maintained topology as a strength in Notre Dame's College of Science. The group is getting a boost by adding faculty through the Advancing Our Vision (AOV), a University-funded, strategic hiring program intended to leverage key areas of research strength. Stephan Stolz, the Rev. John A. Zahm Professor of Mathematics, applied for, and received funding from, AOV to bring on three new faculty members, in addition to two positions offered in the Mathematics Department. There will also be three postdoctoral research positions and four graduate students.

The hires and graduate students are being added over five years to ensure that the best candidates are found. "The AOV program lets you think more long-term and target leaders in the field," Stolz said. "This is a nice thing that enables you to plan, and we've been very successful in terms of hiring very good topologists." So far, three new faculty members have been hired: Professor Andy Putman and Assistant Professors Pavel Mnev and Chris Schommer-Pries. One post-doc is also in place, and graduate students are on the way soon.

"We feel that our recent hires could really help to attract outstanding graduate students in the area of topology and quantum field theory," Stolz said.

Jeffrey Diller, professor and chair of the Department of Mathematics, believes the infusion of new faculty, postdoctoral researchers, and graduate students is adding vibrancy and strength to the program. The dynamic of veteran and new faculty relationships creates an enthusiasm that benefits everyone. "You immediately have a group of people working together, injecting a whole bunch of energy all at once," Diller said. "Topology is a really big part of math these days. This will keep us in the thick of things mathematically."

The AOV award particularly emphasizes connections between topology and physics. "Disciplines have a lot to gain by interacting with other areas," Stolz said. "That's where the really interesting work is happening." ■

College News

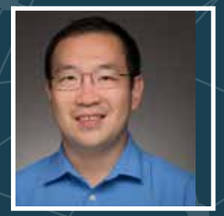
New Faculty

We are pleased to welcome 13 new tenure-track faculty, who joined the College of Science during the summer of 2016.

Three of the 13 are highlighted on page 16.

Jessica Brown
Assistant Professor, Chemistry and Biochemistry
Research: RNA biochemistry and structural biology

Lizhen Lin
Assistant Professor, Applied and Computational Mathematics and Statistics
Research: Big data analysis, including the use of geometry and topology for inference



Xin Lu
Assistant Professor, Biological Sciences
Research: Genetic and molecular basis of cancer progression and resistance to therapy

David Medvigy
Associate Professor, Biological Sciences
Research: Biological ecosystems and atmospheric science

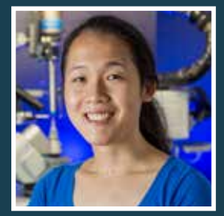
Dong Quan Ngoc Nguyen
Assistant Professor, Applied and Computational Mathematics and Statistics
Research: Problems in number theory having connections to algebraic geometry

Graham Peaslee
Professor, Physics
Research: Experimental nuclear physics, environmental chemistry, and medical isotope harvesting

Marco Radeschi
Assistant Professor, Mathematics
Research: Riemannian and metric geometry

Daniele Schiavazzi
Assistant Professor, Applied and Computational Mathematics and Statistics
Reseach: Application of uncertainty quantification to cardiovascular medicine and the use of numerical models to inform clinical treatment

Cody Smith
Assistant Professor, Biological Sciences
Research: Molecular and cellular determinants of nervous system development, maintenance and regeneration using Zebrafish as a model system



Emily Tsui
Assistant Professor, Chemistry and Biochemistry
Research: Synthetic, inorganic, and surface chemistry, and biomimetic multimetallic clusters and doped semiconductor nanocrystals

Additional faculty hires

Micha Kilburn
Assistant Professional Faculty/ Professor of the Practice, Physics

Sheryl Lu
Assistant Special Professional Faculty, Biological Sciences

Khachatur Manukyan
Research Assistant Professor, Physics

Bahram Moasser
Assistant Special Professional Specialist, Chemistry and Biochemistry

Scott Small
Research Assistant Professor, Biological Sciences

Kelley Young
Assistant Professional Specialist, Chemistry and Biochemistry

Zhenbin Zhang
Research Assistant Professor, Chemistry and Biochemistry

Discoveries lead to new patents

By Gene Stowe

NOTRE DAME SCIENCE RESEARCHERS have received 24 patents in the past five years for their discoveries, including eight patents in 2016 alone. Many of the discoveries focus on potential treatments for illness. The patent rights are assigned to the University of Notre Dame, where the research was conducted, and in the case of outside collaborations, to the other researchers' institutions.

Marvin Miller, the George and Winifred Clark Chair Professor of Chemistry, with more than 20 patents across his career, received two patents this year and one in 2012. One patent has to do with novel drug compounds to treat or prevent tuberculosis or protect plants from fungi. Another drug shows promise in the fight against antibiotic-resistant bacteria. A third compound could fight cancer by inhibiting the growth of cancer cells, such as leukemia, lung, central nervous system, skin, ovarian, renal, prostate, breast, or colon cancer cells.

Steven Ruggiero, professor of condensed matter physics, and Carol Tanner, professor of atomic physics, have been granted two patents in recent years. One involves methods for obtaining information about suspended particles. The other provides methods for quantifying a target material in solution, including detection of a size change of a hybridized nucleic acid complex without the use of nanobeads.

Paul Helquist and Olaf Wiest, professors of chemistry and biochemistry, along with their collaborator Frederick Maxfield of Cornell University received a patent last year for potential treatments for Niemann-Pick Type C (NPC) disease. Included is histone deacetylase inhibitor that has been in clinical trials for two years to assess its value as a therapeutic agent for NPC disease, a rare and fatal genetic disorder. The drug also has potential for treating related disorders. Wiest and his outside collaborators also received a patent in 2013 for treating cancer and blood disorders with drugs fashioned for largazole, a naturally-occurring structure isolated from a blue-green bacterium in the sea.

Bradley Smith, the Emil T. Hofman Professor of Chemistry and Biochemistry, received a patent last year for synthesizing and using croconanine compounds that could be useful for photothermal imaging, photothermal therapy, light-activated drug release, and tissue welding.

In 2012, Smith and a collaborator received a patent for high performance luminescent compounds, dyes that can be used in biological applications.

Mayland Chang, research professor and director of the Chemistry-Biochemistry-Biology Interface Program, and Shahriar Mobashery, Navari Family Professor in Life Sciences, with their collaborator Mijoon Lee last year received a patent for compounds and methods that could treat such conditions as stroke, neurological disorders, and ophthalmological disorders. In 2014, Mobashery and Chang, with their collaborator Dusan Hesek, received a patent for compounds that are especially selective as they fight bacterial infections or inhibit enzyme activity.

Patricia Clark, the Rev. John Cardinal O'Hara CSC Professor of Biochemistry, and her collaborators received a patent for molecular constructs that may be used to examine protein synthesis and protein conformation events, as well as the creation of desired ribosomal displays.

Richard Taylor, professor of synthetic chemistry and Interim Director of the Warren Family Research Center for Drug Discovery and Development, received a patent for antifreeze compounds that could be used for tissue preservation and transplantation, improving the texture of processed frozen food and frozen meats, frostbite protection, crop protection, and green alternatives for land vehicle antifreeze and aircraft deicing.

Steven Buechler, professor in the Department of Applied and Computational Mathematics and Statistics, received a patent for an Accelerated Progression Relapse Test that uses genetic information to gauge whether a person with an illness such as breast cancer would benefit from additional treatment, potentially avoiding unnecessary therapies such as chemotherapy that affect quality of life.

Crislyn D'Souza-Schorey, chair of the Department of Biological Sciences and Morris Pollard Collegiate Professor of Biological Sciences, received a patent for a method for detecting invasive microvesicles derived from tumor cells.

Marya Lieberman, professor of surface chemistry, and collaborators Patrick Flynn of the Department of Engineering and Toni Barstis of Saint Mary's College, received a patent for a Paper Analytical Device (PAD) used to detect low-quality pharmaceuticals.


MARVIN MILLER

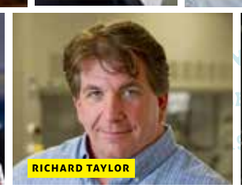

STEVEN RUGGIERO


PAUL HELQUIST


BRADLEY SMITH


MAYLAND CHANG


PATRICIA CLARK


RICHARD TAYLOR


STEVEN BUECHLER


CRISLYN D'SOUZA-SCHOREY


MARYA LIEBERMAN

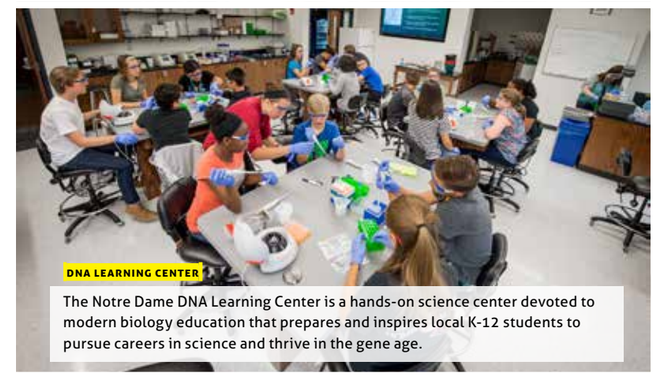
Outreach Initiatives


QUARKNET PROGRAM

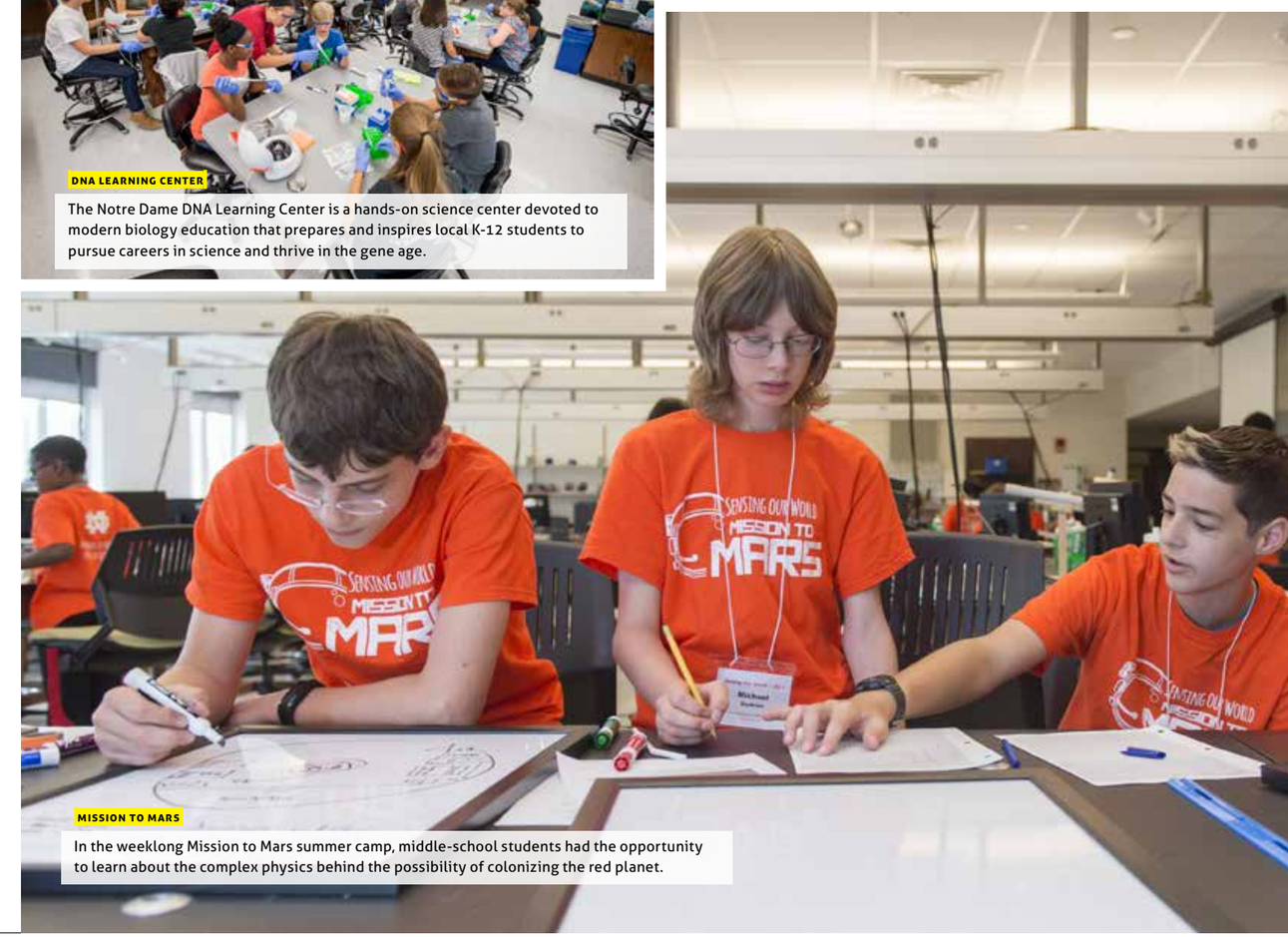
Funded by the National Science Foundation (NSF) and the Department of Energy (DOE), the QuarkNet program seeks to create a national network of science teachers by connecting science teachers with researchers and their work at universities and laboratories around the nation.


EXPANDING YOUR HORIZONS

Through the Expanding Your Horizons (EYH) conference, young girls were able to participate in hands-on activities in science, technology, engineering, and mathematics (STEM) while connecting with STEM professionals in the field who hope to inspire young girls to pursue careers in STEM.


DNA LEARNING CENTER

The Notre Dame DNA Learning Center is a hands-on science center devoted to modern biology education that prepares and inspires local K-12 students to pursue careers in science and thrive in the gene age.



MISSION TO MARS

In the weeklong Mission to Mars summer camp, middle-school students had the opportunity to learn about the complex physics behind the possibility of colonizing the red planet.

NSF Graduate Research Fellowships on the rise

By Mike Westrate and Tammi Freehling

In 2016, the national science foundation (NSF) awarded Graduate Research Fellowships to eight College of Science students, representing one-third of the 24 awards given to Notre Dame graduate students. Another seven earned honorable mentions, of the 17 total for Notre Dame. The NSF-GRFP recognizes and supports outstanding graduate students pursuing research-based degrees in NSF-supported science, technology, engineering, mathematics, and social science disciplines. The award provides a stipend, tuition support, and research funds for three years.

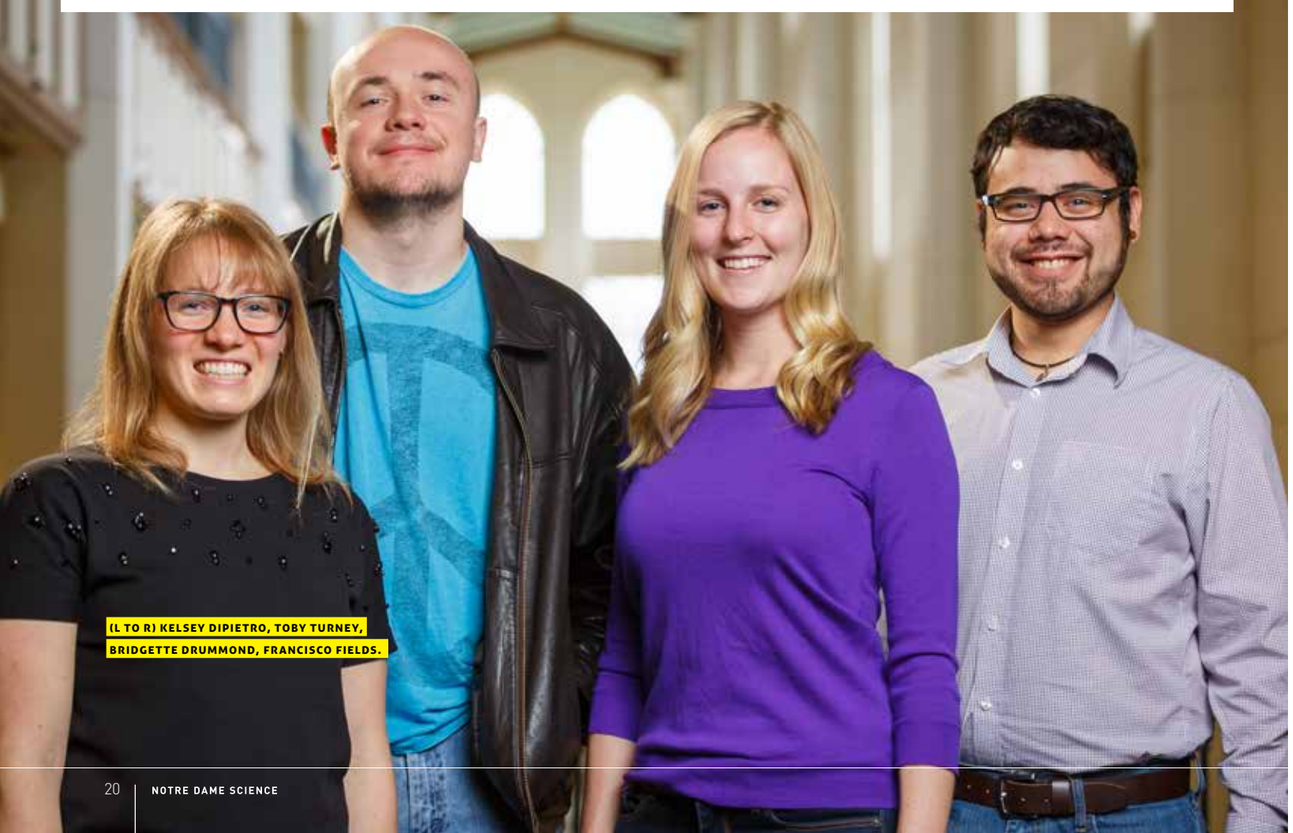
Students create a personal statement and research plan for the fellowship program in conjunction with their advisor and the Office of Grants & Fellowships in the Graduate School. The rise in awards won by Notre Dame students corresponds to the continuing efforts by the Graduate School to provide both one-on-one consultations and group support for students throughout the external funding process, including finding opportunities, writing and revising proposals, and submitting formal applications.

As part of this increased effort, Mike Westrate and his team in the Office of Grants & Fellowships conduct a GRFP summer support program, a fall GRFP workshop series, and an intensive application writing "boot camp" each fall break. All of the graduate-level winners participated in at least one of these specialized events last year. The eight awardees from the College of Science are:

- Kelsey DiPietro, Applied and Computational Mathematics and Statistics
- Bridgette Drummond, Biological Sciences
- Francisco Fields, Biological Sciences
- Heather Forrest, Biological Sciences
- Michael Perlman, Mathematics
- Erica Gonzales, Physics
- Ellen Norby, undergraduate, Biochemistry
- Toby Turney, undergraduate, Biochemistry

The seven honorable mentions from the College of Science are:

- Margaret Regan, Applied and Computational Mathematics and Statistics
- Salvatore Curasi, Biological Sciences
- Martha Dee, Biological Sciences
- Rachel Oidtman, Biological Sciences
- Suzanne Neidhart, Chemistry
- James Quigley, Mathematics
- Zoe Volenec, undergraduate, Biological Sciences



(L TO R) KELSEY DIPIETRO, TOBY TURNEY, BRIDGETTE DRUMMOND, FRANCISCO FIELDS.

Graduate Research

Graduate student Erica Gonzales contributes to rare brown dwarf discovery

By Gene Stowe

Former graduate student Erica Gonzales was conducting her first telescope observations in October 2014 when she helped discover and photograph a rare brown dwarf—an object with a mass between that of stars and planets. Working with her advisor, Justin R. Crepp, the Frank M. Freimann Professor of Physics, Gonzales was able to identify HD 4747B as an important benchmark for studying objects somewhat smaller than stars.

In addition to her discoveries, Gonzales won a National Science Foundation (NSF) Graduate Research Fellowship to continue investigation in the field. Gonzales earned her bachelor's degree at the University of California, Santa Cruz. She came to Notre Dame for graduate school because she wanted to work with Crepp, who leads a new observing program that combines the Doppler method with high-contrast imaging to ascertain the mass of substellar companions using orbital dynamics.

"When I learned of the projects Justin was going to give me, I was excited," she said. "At Santa Cruz, I had worked on theoretical atmospheres of planets. Brown dwarfs are these beautiful objects that fill in the gaps between stars and planets. The smaller of them are very similar to planets. It's something I've fallen in love with."

Gonzales and Crepp went to the California Institute of Technology in October 2014 to conduct observations remotely using the W.M. Keck Observatory in Hawaii. To prepare, Gonzales reviewed Crepp's database of past observations in search of a target and found that they were in the appropriate time frame to observe a suspected companion of the nearby star HD 4747. On the second half-night of observation, they collected information that, upon Crepp's analysis, revealed the brown dwarf HD 4747 B. No other telescope had seen the object previously.

"I am now able to say that I helped discover one of the most important brown dwarfs in our field," Gonzales said, adding that a more recent observation has suggested a possible second candidate. "Justin has taught me a lot about observations and how to be a scientist. We're very fortunate to have access to different techniques that may be combined to make discoveries. This object is going to be very important. It's going to be important to put constraints on how we understand the evolution of planets and cool stars across time." ■

Cancer treatment system wins 2016 McCloskey Business Plan Competition

By Carol Elliott

A novel platform for delivering cancer treatment drugs was the grand prize winner of the 16th Annual McCloskey Business Plan Competition, an annual competition sponsored by the University of Notre Dame's Gigot Center for Entrepreneurship at the Mendoza College of Business.

Certus Therapeutics took home the top prize of $25,000 after competing against seven other ventures during a live event on April 15 at the Mendoza College of Business. Certus makes a liposome product called Lypos, a nanoparticle drug delivery platform with the potential to target cancer cells, lessen the toxic effect of cancer medications, and increase a patient's quality of life.

The winning team was made up of five graduate students representing four academic programs, including business, law, science, and entrepreneurship: Rebecca Shute, ESTEEM '16; Brittany Butler, MS Law '16; Kevin Schneider, MSA '16; Michael Schneider, MSA '16; and Charissa Quinlan, Ph.D. Integrated Biomedical Sciences '18.

The McCloskey Business Plan Competition is intended for traditional entrepreneurial ventures that have not yet been launched or are at the earliest stage of launch. This is typically defined as ventures that have earned less than $500,000 in cumulative revenue, received less than $500,000 in external financing, and have been in operation for less than three years.

All Notre Dame students, alumni, faculty, and staff may compete in McCloskey, which annually awards more than $300,000 in cash and in-kind prizes; however, each team must include a current Notre Dame student who is integrally involved in the business planning process.

The nanoparticle technology underlying Certus' Lypos platform was developed by Basar Bilgicer, associate professor in the Department of Chemical and Biomolecular Engineering. Gaylene Anderson, senior innovation officer for the Cleveland Clinic and Tech Transfer at Notre Dame, advised the Certus team.

A total of 124 teams entered the McCloskey Competition, with 20 teams advancing to the semifinal round on April 14. Eight ventures presented their plans during the live final competition on April 15. Nearly 200 judges and mentors, including members of the Irish Entrepreneurs Network and the IrishAngels Investing Group, worked with the teams to provide feedback and guidance. ■

Could you describe your thesis in three minutes?

By Marissa Gebhard

AT THE 2016 THREE MINUTE THESIS competition (3MT), three College of Science graduate students competed with six other Notre Dame graduate students for prize money and a bid to the regional championships. Nicholas Myers in the Department of Chemistry and Biochemistry won second place ($1,500) and Claire Bowen in the Department of Applied and Computational Mathematics and Statistics won the People's Choice Award ($1,000).

The competition challenges graduate students to explain their research in clear, succinct language in just three minutes. The students are allowed only one slide at the competition. Myers said, "I realized how difficult it is to create an effective graphic that a person can quickly interpret."

Myers educated the crowd on the devastating problem of counterfeit and low-quality medicine in the developing world. "I talk to a lot of non-chemists, so I have to sell my ideas in a way that is easy for them to digest," Myers said. "The most challenging aspect is avoiding over-generalizing my research while still using non-technical rhetoric. Having only three minutes to summarize my entire thesis, I made sure every spoken phrase had meaning and every visual display could be quickly understood. Conveying ideas succinctly is an important skill in any career."

Through her presentation, "Big Brother in Big Data," Bowen shared her work on an algorithm that provides a high level of privacy protection for media users and online consumers while preserving the statistical structure of big data sets for researchers, corporations, and government agencies. Her research addresses confidentiality issues of big data. ■

NICOLAS MYERS developed paper test cards that can identify low-quality pharmaceuticals effectively and inexpensively.

Graduate Student Spotlight

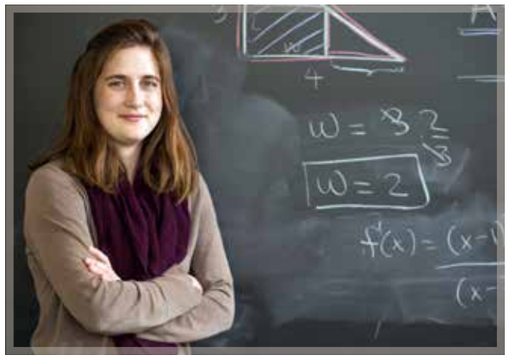
* * * *

Laura Wells

By Gene Stowe

LAURA WELLS, A THIRD-YEAR PH.D. STUDENT IN THE DEPARTMENT of Mathematics who came from Providence College, has earned praise from both students and department colleagues for her engagement and dedication. She has an Arthur J. Schmitt Leadership Fellowship.

"She's an amazing teacher," said Wells' adviser, Stephan Stolz, who has co-taught with Wells. "Whenever she gives a talk, it's very clear. She's a great communicator, has a very nice personality, and broad interests.



Wells, whose interest in mathematics began with high school calculus and was further sparked by inspiring professors she encountered in college, studies quantum field theory. The interdisciplinary area seeks to describe physics in a mathematical framework, translating between geometric and algebraic models to leverage the power of computing.

"She's been a great graduate student during her three years here—she's very engaged in the department," said Peter Cholak, director of Graduate Studies. "She was chosen by the other TAs to be the TA coordinator. She's done a great job in the classroom for us, and she's been a great leader for us and our graduate students."

Wells, also was accepted into Notre Dame's doctorate program in philosophy but chose math. She has a broad interest in interdisciplinary learning and hopes to have a career as a professor at a liberal arts university. ■

Graduate alumnus leads IBM research team in South Africa

By Cliff Djajapranata

AFTER COMING ALL THE WAY FROM KENYA, GEOFFREY SIWO received his Ph.D. in biological sciences from the University of Notre Dame in 2014. Not even three years later, he has found himself across the world again, this time in Johannesburg, South Africa, as a research scientist at IBM Research Africa leading the Data Driven Healthcare team in its latest research endeavors.

At IBM, Siwo's research involves seeking solutions to problems in biology and clinical medicine by integrating biological data and evolutionary principles with statistical, computational, and artificial intelligence technologies. "While at IBM, my research has led to a new computational approach for mining biological networks to find hidden connections between cancer-initiating genes and genes that drive the spread of cancer cells around the body, which could provide clues to new personalized cancer therapeutics," Siwo said. And he is not working alone—Siwo is just one of IBM's 3,000 researchers fanned out across 12 laboratories around the world with whom he is able to collaborate and share information.

Siwo gave credit to Notre Dame and his Ph.D. advisor, Michael Ferdig, a professor of biological sciences. "His leadership and enthusiasm in the genomic and evolutionary biology of the human malaria parasite made me extremely eager to join his lab at Notre Dame," Siwo said. "Even long before I applied to Notre Dame, we had many open conversations about his research and views on how biological species evolve over time and whether this could be predictable." He said that Notre Dame taught him to be unafraid to question assumptions that are taken for granted to be true. "By the time I graduated from Notre Dame, I had become a better researcher and had learned to work with diverse teams in high risk ideas for my Ph.D. research."

Looking ahead, Siwo hopes to make advances in the field of biomedicine, as it is still difficult to deliver effective and affordable medicine. According to Siwo, creating new pharmaceuticals often takes too long. "The world is largely unprepared for new disease outbreaks, and contagious pandemics could have a devastating impact across the globe," Siwo said. "My long-term goals are to develop technologies for accelerating the speed at which new medicines, vaccines, and diagnostics could be discovered and made available to those who need them." ■

GEOFFREY SIWO (L) WITH IBM'S CEO GINNI ROMETTY

Photos provided by IBM Research

The newest major is already the largest

By Cliff Djajapranata

THE NEUROSCIENCE AND BEHAVIOR MAJOR is one of the fastest growing majors at the University of Notre Dame. Nancy Michael, assistant teaching professor and director of undergraduate studies for the major, advises approximately 215 neuroscience students in the College of Science. It is the now the largest major in the college.

One of the main attractions of this relatively new major is the flexibility it offers graduates in this field of study. Students can take courses ranging from nanotechnology to policy development. This diversity leads to a wide array of options post-graduation. "There is a lot of opportunity in the major to pick and choose what areas interest you and really develop a background in various aspects of the field. For example, you can focus more on psychological aspects of neuroscience like personality development or more on biological aspects like the mechanisms behind hunger," junior neuroscience major Kelly Heiniger said. While a majority of neuroscience students go on to medical school, others find just as much success in business school, law school, or graduate school in pursuit of a Ph.D, and just as many others find success in rewarding careers right out of their undergraduate years.

Michael said that students discover that they have chosen the right major when they find themselves enjoying both their psychology classes and courses that give a cellular understanding of behavior patterns. "I'm also drawn to neuroscience because it has really changed how I understand basic biological processes. Because of my neuroscience courses, I now understand the biology, molecules, and mechanisms behind hunger and satiety—an area I find really intriguing," Heiniger said. And this dual knowledge can be applied anywhere because, according to Michael, a better understanding of the brain and behavior is applicable to just about any field.

Through non-traditional course structures, such as community-based learning and research, as well as community engagement opportunities, the neuroscience and behavior major offers many opportunities for students to process the information they learn in their courses in a different way. Students can choose to work with various community partners in South Bend, including the Boys and Girls Club, the Robinson Community Learning Center, and the South Bend Center for the Homeless.

Ultimately, Michael hopes that the neuroscience program will help develop good citizens by empowering students to apply what they learn in the classroom to the real world. Doing so in a human way will have a broad impact in the communities the graduates serve. ■

KELLY HEINIGER is a junior neuroscience major.

Making applied physics engaging

By Gene Stowe

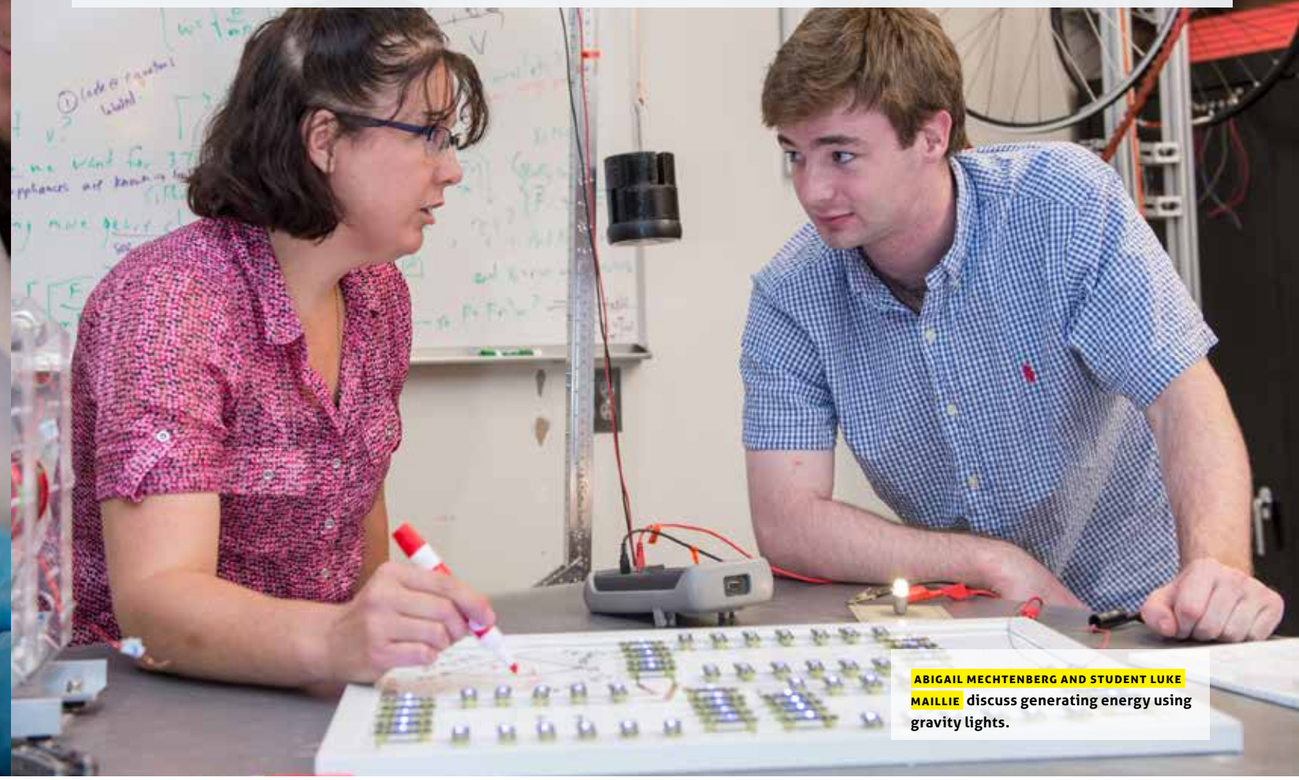
AFTER A STINT AT COLGATE UNIVERSITY, Abigail Mechtenberg came to Notre Dame as an assistant teaching professor with a laboratory that engages undergraduate students in research.

Mechtenberg brings an "experimental design" approach to the physics curriculum laboratory that helps students advance from the old "cookbook" replicating method to emerging "inquiry-based" models across six weekly labs plus a long-term project. The strategy engages students and makes applied physics vivid for them.

"The students are more in control of the types of research questions and hypotheses they generate or are interested in," Mechtenberg explained. They are more engaged in error analysis, uncertainty, and big-picture thinking." For example, students can take an experiential path by analyzing gravity lights that generate energy from falling weights, gears, magnets, and coils, or they can take a more theoretical path by evaluating the physics of movie or video game simulations. Physics 2 students can study alternatives such as solar panels, concentrating solar power, wind, hydroelectricity, biodiesel, biogas, biomass waste incineration, or microgrids in general.

Mechtenberg mentors undergraduate students who are interested in conducting research. She focuses on designing electricity systems for extreme conditions, such as power outages during storms or locations that are not served by reliable grids. Two students joined her lab after she gave a talk at their sophomore physics seminar. One focused on a sustainable tech project, generating on-site energy through gravity lights, the falling-weight systems that she uses in students' labs. Another student chose a high-tech project, a "smart grid" system that responds to consumers energy usage, and had a paper published in a journal of the Institute of Electrical and Electronics Engineers.

Students also participate in many of Mechtenberg's projects in Africa, a set of initiatives she calls Empowering Ugandans to Power Uganda. On a recent visit to Uganda, she worked with local experts to improve infrastructure with two new wind turbines, a new hydroelectric generator, an upgrade to another hydroelectric generator, redesigns for a concentrated solar power generator, a thermoelectric cook stove, an energy-generating waste incinerator, an evaluation of the gravity light, and work on biogas and biodiesel generators–all part of an E3 (Education, Engineering and Entrepreneurship) pipeline that moves physics knowledge through design iterations to business ventures. For example, another student is planning to open a business energy incubator this summer in Fort Porto, Uganda, to help develop business models for people to market the energy they are not using in their businesses. ■



ABIGAIL MECHTENBERG AND STUDENT LUKE MAILLIE discuss generating energy using gravity lights.

Undergraduate News

Undergraduates engage in funded summer research

By Tammi Freehling

EACH SUMMER, THE COLLEGE OF SCIENCE SUMMER Undergraduate Research Fellowships (SURF) provide opportunities for Notre Dame sophomores and juniors to engage in research. With support from donors, and in collaboration with the Center for Undergraduate Scholarly Engagement, Indiana University School of Medicine–South Bend, and Glynn Family Honors program, students participate in full-time research for nine-to-ten weeks and are mentored by College of Science faculty or international collaborators at an institute abroad. More than 60 students participated this summer, four of who are featured below.

Like all students who participate in SURF, **TIFFANY TONI**, a student in the Department of Chemistry and Biochemistry, is grateful to the donors who make SURF possible. She said of her research experience this past summer, under the mentorship of Associate Professor Brandon Ashfeld, "It allowed me the chance to focus primarily on my research, which unfortunately is not possible during the school year. I was able to make a lot of progress in the research, as well as developing my own skills as a chemist."

"I enjoyed being able to work independently on the day-to-day operations. I greatly enjoyed my experience this summer and would definitely recommend COS-SURF to anybody interested in research."
—Anthony Nguyen

Under the advisement of Research Associate Professors John Grieco and Nicole Achee, **ROBERT WOZNIAK** traveled to Belize to complete his research experience. There they addressed several unanswered questions regarding the current preventative measures used to combat Chagas disease. His team searched for Triatoma dimidiata (commonly known as kissing bugs), one of the transmission vectors of Chagas disease. They set odorant bait traps to determine if the odorants could successfully stimulate the bugs' olfactory system and improve capture efficiency. The team also explored various caves across Belize to collect wild type T. dimidiata. Wozniak said. "We then investigated the repurposing of a chemotherapeutic agent, miltefosine, for Chagas disease treatment to determine its potency against the parasite and transmission vector. The final part of our research was to find how new treatment methods, such as miltefosine, could potentially be implemented into the Belizean health system by interviewing various health professionals, including pharmacists, physicians, and members of the Belize Ministry of Health and Department of Health Services."

XIAOYU YU studied mosquito species and behaviors with the goal to prevent malaria. Her team in Neil Lobo's laboratory worked on 330 mosquito samples from the Democratic Republic of Congo (DRC). With dissection and sequencing, they were able to identify the species of the mosquitoes on a molecular level. Her team found four new species in the process. She said, "I had a great time, everyone working in the lab was really helpful—they were always there for me when I had questions or needed troubleshooting. I am studying abroad this semester, and I will definitely go back to the Lobo lab when I return next semester."

ANTHONY NGUYEN worked under the guidance of Assistant Professor Zain Syed studying the influence of endogenous mosquito microbiota on circadian rhythm behavior. He said, "I enjoyed being able to work independently on the day-to-day operations. I greatly enjoyed my experience this summer and would definitely recommend COS-SURF to anybody interested in research." ■


TIFFANY TONI


ROBERT WOZNIAK


XIAOYU YU


ANTHONY NGUYEN

Savannah Kounelis receives Fulbright award

By Chontel Syfox

SAVANNAH KOUNELIS

SAVANNAH KOUNELIS OF PORTAGE, MICH., GRADUATED FROM the University of Notre Dame in May 2016, with a bachelor of science degree in neuroscience and behavior. She is a recipient of the prestigious Fulbright study and research grant, which has allowed her to conduct research in Belgium during the 2016–17 academic year.

Hopes of better understanding the mechanisms that drive brain disorders, such as mental illness and disease, inspired Kounelis to pursue an education and career in neuroscience. Her particular area of interest is neuroplasticity, or the brain's capacity to change its functional and anatomical organization by forming new synapses and pathways. The process of neuroplasticity happens naturally throughout the human lifetime in response to environmental, behavioral, and neural changes, but it may also happen to compensate for function loss after traumatic brain injuries. Understanding the mechanisms underlying neuroplasticity is, therefore, crucial to the prevention and reversal of degenerative processes in the brain.

Kounelis was awarded the Fulbright grant to carry out research examining neurodegeneration within the hippocampus and cortex of the brain resulting from the malfunction of the protein matrix metalloproteinase 3 (MMP-3). The study she is executing uses a model of induced neurodegeneration in mice, in order to characterize morphological changes in the hippocampus and cortex resulting from the loss of MMP-3. The study also aims to identify how the loss of this protein impacts cognitive functions associated with these brain regions. Her work will not only advance the understanding of how MMP-3 is implicated in the healthy development of these brain areas, but it may also increase understanding of how MMP-3 deficiency leads to diseased brain states similar to those seen in patients suffering from Alzheimer's disease.

With the help of the Fulbright grant, Kounelis has been uniquely positioned to conduct her research in the neural development and animal physiology laboratory of Lieve Moons at the University of Leuven, one of only a handful of labs worldwide exploring the relationship between matrix metalloproteinases and neurodegenerative diseases. "I have the opportunity to interact with researchers and students from all over the world in a highly collaborative lab, in which I am able to pursue novel techniques not available to me previously." Kounelis said, adding, "I have already learned and encountered so much."

Upon completion of her research year at the University of Leuven, Kounelis intends to continue her research in neurobiology and neurodegenerative diseases by pursuing an M.D./Ph.D, and her ultimate goal is to become a physician scientist. She stressed how invaluable the Fulbright is to her future in the academe saying, "The Fulbright has allowed me to pursue graduate courses in the biomedical sciences, while also doing research related to neurodegenerative diseases. The academic and work culture surrounding research here differs from that in the U.S., and it is magnificent to be able to conduct research in a new environment at a top research university in Europe." ■

(L TO R) MADELINE ZUPAN, KATHERINE MCINTYRE, AND ROLAND REBUYON

Snapchat leveraged to "Snap Out of Sickle Cell"

By Tammi Freehling and Cliff Djajapranata

LAST SPRING, A TEAM OF TWO NOTRE DAME SCIENCE SENIORS and one Notre Dame engineering senior was awarded the second prize in the Sickle Cell Disease Challenge for Undergraduate Students sponsored by the Department of Health and Human Services (HHS) National Heart, Lung, and Blood Institute at the National Institutes of Health (NIH) in Bethesda, Md. For their efforts, the team won $5,000 plus travel expenses to attend the Annual Sickle Cell Disease Clinical Research Meetings in Bethesda this past August.

At the conference, the team, led by Madeline Zupan and joined by Katherine McIntyre and Roland Rebuyon, presented and demonstrated its winning entry titled "Snap Out of Sickle Cell: Informing and Involving America with a Targeted Social Media Campaign." The team's project leverages the popular social media image-sharing platform, Snapchat, to disseminate information about sickle cell disease by using geofilters (graphics that overlay images) that will offer useful facts and information about the deadly disease. The team, mentored by Professor Kasturi Haldar, hopes to use its geofilters on June 19, World Sickle Cell Awareness Day. "We created the idea of using Snapchat as a tool to engage and inspire the next generation of researchers to improve the lives of those living with sickle cell disease," McIntyre said. "According to our demographic research, 92 percent of college students use Snapchat every day, so we found it an intuitive way to reach our intended audience."

Zupan added that the team's work was well received by clinicians and researches at NIH and other sickle cell advocates. Because of the conference, the team has been connecting with a few rare disease initiatives, including one in Indiana. "Because our tool is engineered to target the Millennial demographic, many of our collaborators are interested in using it to capture the attention of a traditionally disinterested cohort," Zupan said.

Since the conference, the team has been in touch with the Rare ND Club on campus, which is considering utilizing the geofilters. "I am so happy to see the outstanding efforts by students and researchers here. In the true spirit of Notre Dame, many are working to champion rare disease patients," Zupan said.

Wherever the project goes from here, Zupan believes she has learned a lot and hopes that the project can expand to other rare diseases. "We have learned not only to strengthen our own personal skill sets in science and engineering, but also to work productively in teams to address challenges that national organizations such as the National Institutes of Health must confront daily," Zupan said. "Should the launch prove successful, it is a platform that is replicable for all other 7,000 rare diseases that exist in the United States. This is a powerful and effective tool that can inspire others to engage in important discourse about rare or neglected diseases." ■

Math majors discover research in summer program

By Gene Stowe

TWO YEARS AGO, MATHEMATICS PROFESSOR Jeff Diller created a summer math program for freshmen and sophomores at Notre Dame to accelerate their progress in mathematics. The program consists of a combination of individual projects, group sessions, mentoring, and weekly presentations. With support from the College of Science, the program engages 10 students a year, including talented scholars from Notre Dame and other universities.

"We get a lot of good students," said Diller, who ran the mathematics honors program for three years and is now chair of the Department of Mathematics. "I'm very concerned about giving them the chance to pursue math on their own outside the classroom."

Junior Paul Sweeney, winner of the 2014/15 Aumann Prize for First Year Students in Mathematics, said the summer course helped advance his plan to go to graduate school in mathematics.

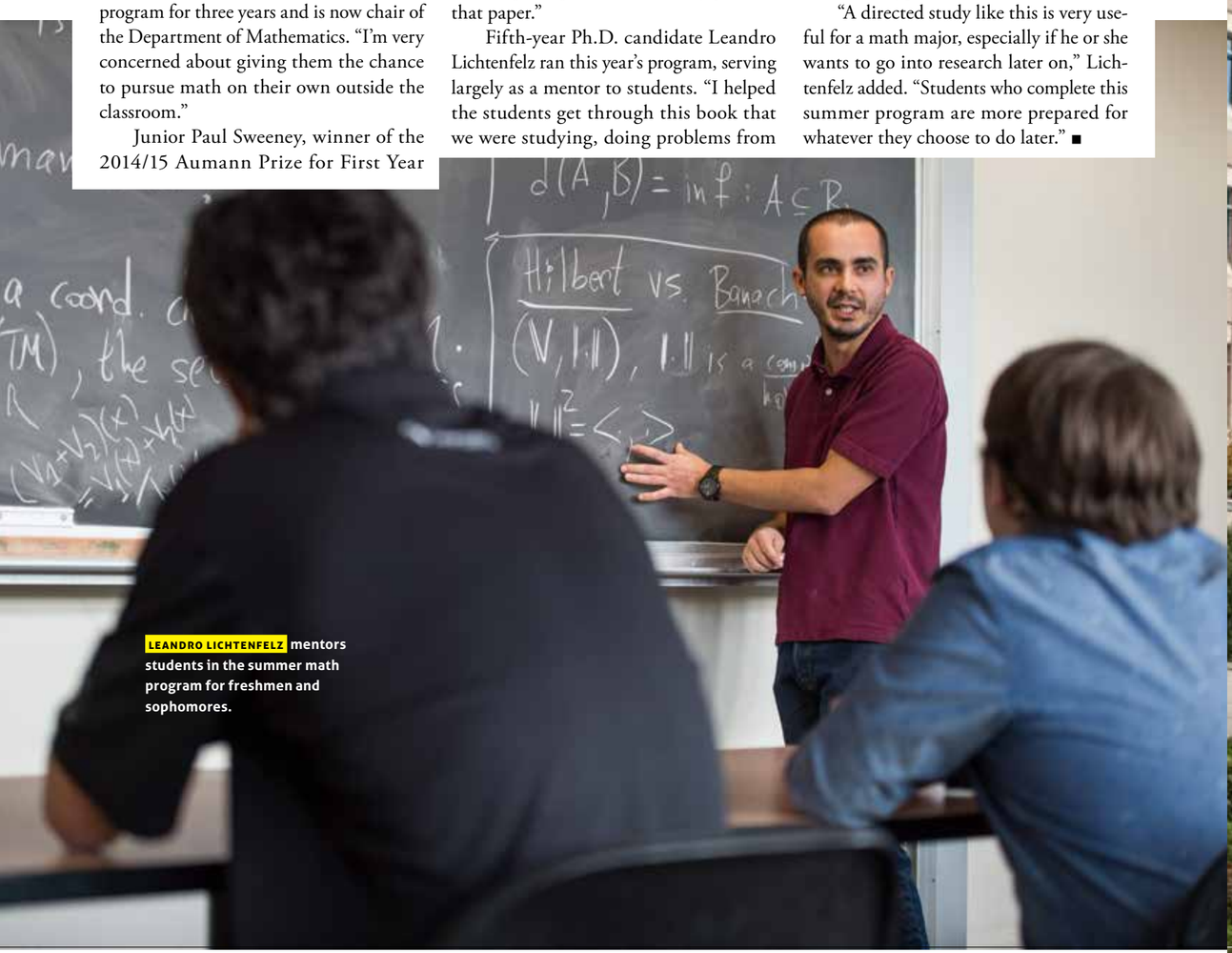
"I knew that I wanted to do something math-related over the summer," he said. "I'm thinking about going to grad school. This would help me understand math research—what researchers actually do. Every day in the morning we met. We discussed topics from the textbook *Convexity* by Roger Webster. In the afternoon, we focused on more individual research."

Sweeney ended up writing a paper proving Croston's Formula. "The course taught me how to write a math paper. It was a big thing for me to actually produce that paper."

Fifth-year Ph.D. candidate Leandro Lichtenfelz ran this year's program, serving largely as a mentor to students. "I helped the students get through this book that we were studying, doing problems from each section, and understanding the material thoroughly," he said. "Sometimes they would have questions that weren't covered by the book or questions on things that weren't so clearly explained in the book, and I helped them with those. I believe I was also able to give them a broader perspective, big picture view of things, which is easy to miss when you first encounter a new subject in math."

The structure and content of the program give the students a head start in their academic careers, Lichtenfelz said, adding that convexity is an important subject in pure and applied mathematics that is rarely covered in typical courses.

"A directed study like this is very useful for a math major, especially if he or she wants to go into research later on," Lichtenfelz added. "Students who complete this summer program are more prepared for whatever they choose to do later." ■



LEANDRO LICHTENFELZ mentors students in the summer math program for freshmen and sophomores.

Undergraduates advance their research skills at MD Anderson Cancer Center

By Tammi Freehling

FOR SIX COLLEGE OF SCIENCE STUDENTS, SUMMER "BREAK" MEANT advancing their research skills at MD Anderson Cancer Center in Houston, Texas. The students' experiences were funded by Notre Dame through the generosity of a donor.

The University of Notre Dame Summer Undergraduate Research Program at MD Anderson Cancer Center is a competitive, ten-week program designed for outstanding and highly motivated Notre Dame undergraduate students interested in pursuing a career in cancer research. Dominic Chaloner, research associate professor and undergraduate research coordinator, explained that the selected students have the opportunity to participate in "cutting-edge research" at what is known as "one of the top centers for cancer research in the country, if not the world." The program offers undergraduate students the opportunity to gain hands-on experience that simply cannot be replicated in a classroom or teaching lab. Following, four seniors and two juniors share what they learned from their experiences.

Notre Dame student, KATHRYN TIGHE during her summer internship at MD Anderson.

KATHRYN TIGHE, a junior neuroscience and behavior major, worked on research to investigate the timing of mitochondrial DNA replication relative to the cell cycle. About her experience she shared, "I thought I knew what to expect, having taken several biology lab courses, but now I know that nothing quite compares to the real thing. I have learned so many new techniques this summer and have improved the skills I learned at school. While my mentors were very hands-on and willing to explain their rationale and procedures, they also gave me considerable independence, which has been invaluable for not only widening my skill set, but also bolstering my self-confidence."

MAGGIE (ZHENYUE) ZI, a senior biochemistry and applied math dual major, worked on the computational analysis of glioma, or brain tumors. About her experience she said, "I even went inside an operating room for the first time and experienced what is involved in being a surgeon. Being able to visualize the many ways that I can help people as a doctor felt really amazing. [I have] grown so much as a researcher and become more determined to become a doctor."

AMY WANG, a senior preprofessional studies major, conducted research to identify the biological consequences of chronic stress in colon epithelium. Wang said her mentor, Dr. Dorniak, "provided guidance with performing the different techniques needed for my research, but he also allowed me the independence to perform the techniques on my own. The experience has given me greater confidence in my skills as a researcher and reassured me of my interests in the clinical field as it applies to medicine."

DAN MCKEE, a senior science-business major, researched the protein expression patterns in triple-negative breast cancer tissues. McKee said, "The goal of these analyses is to detect molecular differences between the tumor before treatment and the residual tumor after [treatment with chemotherapy]. The differences that are found can help highlight potential reasons for the survival of some cells after chemotherapy." McKee said of his experience, "Being able to comprehend a problem and logically work through a set of steps to create a solution is imperative to succeeding in research and medicine. My immersion into research this summer taught me more about how to find solutions and stay determined when you appear to have reached a dead end."

BRAD MARTIN, a junior neuroscience and behavior major, worked in a lab that primarily studies the role of the tumor microenvironment in the early metastasis of lung cancers. "I have been extremely lucky to have a great research mentor. Even with the techniques that I have had previous experience with, she has helped me understand them to much greater level. I now know and understand the reasons behind specific methods but also how scientists think about their research and experiments. I know I am learning from some of the best cancer researchers in the world," Martin commented about his experience.

MATTHEW GOBLIRSCH, a senior chemistry and philosophy major, studied microRNAs in cancer and sepsis. Goblirsch shared about his experience, "As someone who never had much time during the semester for research, these two summers have been very important for me in developing my understanding of, and appreciation for, life in a laboratory. There were challenges, but we dealt with the issues as they came up. In fact, I now appreciate the challenges much more than the successes because I gained more skills in working through the difficulties than I ever could gain if things always went well and according to plan." ■

Active learning at Cold Spring Harbor

By Cliff Djajapranata

RESEARCH CAN BE A BIG PART OF BEING AN UNDERGRADUATE student at the University of Notre Dame. One of the premier programs is a result of a partnership between the University and the prestigious Cold Spring Harbor Laboratory (CSHL) in New York.

Hailed as "one of the most innovative institutions in the U.S. for specific areas of biological research" by Dominic Chaloner, research associate professor and undergraduate research coordinator for the College of Science, CSHL has a special partnership with Notre Dame that reserves one Notre Dame student a spot every summer to conduct research; however, in past years, Notre Dame has sent two students to the esteemed research institution.

Hearing from his mentors and colleagues that CSHL was the "mecca for biology," senior Daniel Barabasi was one of two Notre Dame students to go to CSHL in summer 2016. "At Cold Spring Harbor, I worked on an analysis pipeline for neural imaging. My mantra for my research goals has become 'capturing biological complexity with theoretical simplicity,'" Barabasi said. "Having the opportunity to work directly with experts in neuroscience allowed me to explore the thought process behind experiments in the field, which I will use to feed back into my analytical work."

Junior Ashley Kyalwazi also went to CSHL last summer to conduct neuroscience research. "I completed a ten-week research project with the goal of developing a model that would enable me and others who would come after me to study a particular network of inhibitory neurons in the auditory cortex of surrogate mice," Kyalwazi said. "I was very interested in the work I was doing because the auditory cortex plays a major role in social communication and learning, in both mice and humans."

Chaloner explained how the opportunity at CSHL is unique in that it offers a realistic and authentic research experience that just is not possible in the traditional classroom lab. "Undergraduate research is a very active way of learning, and that's the way we should teach." ■

Student Athlete Spotlight

* * * *

Eva Niklinska

By Grant Johnson

EVA NIKLINSKA IS A SENIOR IN THE Department of Preprofessional Studies focusing on biology and anthropology. Her passion for people and her zeal for science shaped her desire to become a physician, with a focus on community and global health. In addition to her many research accomplishments and maintaining a 4.0 GPA, Niklinska is also an accomplished Notre Dame athlete.

Niklinska is a member of the Notre Dame fencing team, where she was named the women's epée captain this year. Over the course of her athletic career, she's received many other honors, including selection into the 2016 All-ACC Academic Team, the 2016 Polly DeCicco/Georgette Auriol Women's Epee Leadership Award, and the 2016 Community Champion Award, which recognizes the contributions of Notre Dame student athletes who embody the spirit of leadership, commitment and selflessness. Outside of her academic and athletic life, Niklinska gives back to the South Bend community where she grew up. Throughout the year, she volunteers at the Sister Maura Brannick Health Center, a clinic that provides primary healthcare services to uninsured residents of St. Joseph County. It is here that Niklinska continues to better herself and her understanding of the healthcare system by engaging with a diverse and, sadly, often marginalized population in her community.

Niklinska has been accepted to many prestigious medical schools: Pritzker School of Medicine at the University of Chicago, Vanderbilt, Duke, Harvard, Stanford, Yale, Northwestern, Johns Hopkins, University of Pittsburgh, Virginia, and Indiana University.

Young Alumnus Spotlight

* * * *

Charles Cong Yang Xu

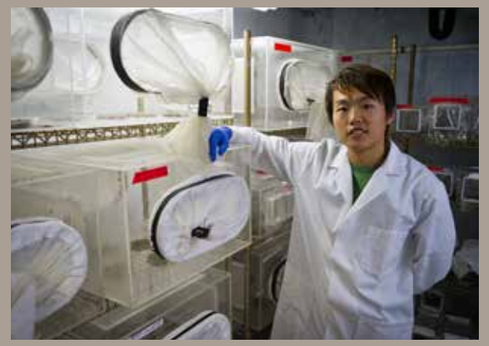
By Cliff Djajapranata

WHEN HE WAS A STUDENT AT THE University of Notre Dame, alumnus Charles Cong Yang Xu '14 found a novel and promising source of noninvasive spider and insect DNA by extracting the DNA from spiderwebs.

Today, Xu is a Ph.D. candidate at McGill University, where his research revolves around experimental genomics of deer mice and freshwater microbes. While his Ph.D. research no longer involves spiders, Xu has taken on a little side project in the Bahamas, exploring the viability of collecting spiderweb DNA from the wild, which contrasts with his previous experience of collecting spiderweb DNA in a controlled setting. He also hopes to compare spiderweb DNA and DNA collected from spider guts to see how well spiderweb DNA reflects the local insect community by comparing with other traditional sampling methods like Malaise traps.

As an environmental science major at Notre Dame, Xu said he had the idea of uncovering the DNA of spiders while he was studying environmental DNA of fish in the lab of David Lodge, formerly the Ludmilla F., Stephen J., and Robert T. Galla Professor of Biological Sciences. He says these research experiences at Notre Dame helped him think more broadly when doing science.

While at Notre Dame using web samples from black widow spiders fed with crickets, Xu and his collaborators successfully used DNA samples to identify both the spider and the species of its prey. Such noninvasive sampling to obtain genetic information could have practical implications in several fields, including conservation research and pest management.



Xu pursues interests across diverse fields of ecology and evolution. "I would say my research interests lie at the intersection of genetics and the environment, whether it's in evolutionary biology to use genetics to study how the environment causes organisms and populations to evolve, or in a more applied context such as conservation genetics." Xu completed a two-year Erasmus Mundus Master Programme in Evolutionary Biology at Uppsala University in Sweden. He also has plans to conduct sampling at the Morgan Arboretum in Montreal this summer.

Faculty Spotlight

Amanda Hummon

Basic science, in the lab and the classroom

By Brian Wallheimer

In the lab, Amanda Hummon is working to improve patient outcomes by addressing significant questions about how cancer cells and the drugs used to treat them work.

A patient with stage 3 or stage 4 colorectal cancer is likely to have surgery and receive chemotherapy treatment to guard against metastasis. Someone with stage 2 cancer probably won't go through those same treatments, but it doesn't mean the cancer won't come back or spread.

Hummon, an associate professor in the Department of Chemistry and Biochemistry, tracks protein and gene expression, as well as other molecular markers, to determine when surgery isn't enough for stage 2 colorectal cancer patients.

"Looking at molecules and gene expression patterns can help predict whether or not the cancer will return," Hummon said. "In patients where there will be a recurrence, it would be advantageous to go through chemotherapy."

Another project includes developing approaches to evaluate chemotherapy drugs. Sometimes, a tumor doesn't have an adequate blood supply and drugs meant to kill cancer cells cannot get to their targets. Or the drug isn't metabolized, a key step in turning on its ability to kill cancer cells.

Using 3-D cell cultures that mimic tumors, Hummon analyzes the drugs through mass spectrometry to see whether they are finding their way to a tumor, and whether those drugs are being metabolized. Her laboratory can determine the mass of the molecules and how that mass changes to understand how and if cancer cells are effective.

Hummon is also uncovering the cellular changes that occur when some people fast before chemotherapy treatments. The short-term starvation seems to alter cellular signaling pathways, making chemotherapy more effective.

Her laboratory uses 3-D cell culture mimics to better understand autophagy, the degradation and recycling of cellular materials. Again, using mass spectrometry, Hummon can determine which proteins are altered when cells are starved, potentially shedding light on targets that improve drug efficiency.

When she's not in the lab, Hummon has particularly enjoyed teaching Chemistry 101, a class geared toward non-science students who need to fulfill graduation requirements. She sees the class as a challenge since most students aren't initially interested in science.

Hummon has developed 38 lesson plans, all around different molecules, including lessons on how those molecules have played important roles in the history of the world. She does in-class demonstrations, such as using liquid nitrogen to make ice cream, to make the class fun. By the end of the semester, she hopes to find students who see the value and importance of science in their daily lives.

"Within this cohort of students, a lot of them are going to do other things in life, so it's really important that they appreciate science in our society," Hummon said. ■

Faculty Spotlight

Jonathan Hauenstein

Applied mathematician applies his Notre Dame education to teach the next generation

By Gene Stowe

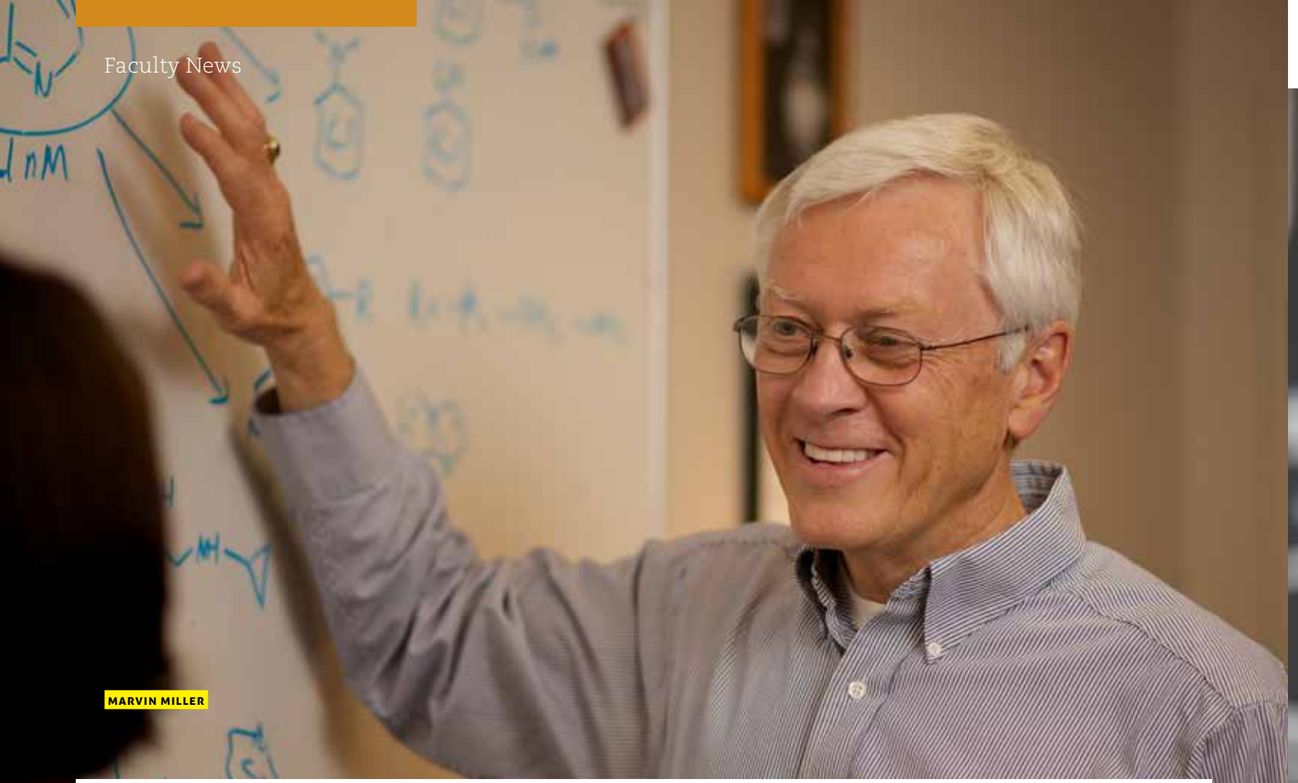
While studying for the Ph.D. he earned in 2009 under advisor Andrew Sommese, Jonathan Hauenstein found his research focus—how to solve general classes of nonlinear systems. Hauenstein learned teaching skills and best practices at the Kaneb Center for Teaching and Learning.

Hauenstein, who worked after graduation at the Fields Institute in Toronto, Texas A&M University, the Institut Mittag–Leffler in Sweden, N.C. State University, and the Simons Institute for the Theory of Computing in Berkeley, Calif., returned to Notre Dame in 2014. He is an associate professor in the Department of Applied and Computational Mathematics and Statistics (ACMS), where Sommese is chair.

Hauenstein's teaching repertoire includes a course on numerical analysis for first-year graduate students, probability for sophomores and juniors, and a topics course on solving nonlinear equations that he created for seniors. This range allows him to encounter students at different stages of growth. "You see people early on, sophomores, and as they go through their years here at Notre Dame, you see them advance to higher level courses. By teaching numerical analysis, you get to impart a positive impression of computational and applied mathematics on first-year graduate students."

That impression incudes regular reference to his own Notre Dame experience. "I catch myself saying often, 'when I was a graduate student here,'" Hauenstein said, adding that he encourages students facing challenges such as midterm exams. "They're starting to feel overwhelmed. I can help them understand that this is a fleeting moment. It'll pass and things will be much better. I look back at the courses I took, and I can really help students understand what is the main material in that course that's going to help them going forward, 'from my experience, this topic in that course was very important and has turned into these other ideas.' I try to emphasize in the courses that I teach that these are the places I found really important and helpful."

"I had no doubt that Jon would have an excellent career," Sommese said. "He is one of the best applied mathematicians of his generation. He has so many grants and awards, including, a Sloan Research Fellowship, DARPA Young Faculty Award, Army Young Investigator Award, and Office of Naval Research Young Investigator Award. Jon already is playing a key role in ACMS. He has a very bright career." ■



MARVIN MILLER

Marvin Miller inducted into the ACS Division of Medicinal Chemistry Hall of Fame

By Tammi Freehling

MARVIN MILLER, PH.D., WAS SELECTED FOR INDUCTION INTO THE American Chemical Society (ACS) Division of Medicinal Chemistry (MEDI) Hall of Fame during the ACS 252nd National Meeting and Exposition in Philadelphia in 2016.

For nearly 40 years, Professor Miller has made countless contributions to medicinal chemistry, focusing on a mixture of synthetic organic chemistry and bioorganic chemistry, to develop new methods to study, prevent, and cure disease, particularly tuberculosis and bacterial infections.

Professor Miller has more than 300 peer-reviewed publications and more than 25 U.S. patents. A popular lecturer across the country and around the world, he has mentored more than 80 graduate students and 70 postdoctoral researchers and visiting scientists. On nominating Miller, Shahriar Mobashery, Ph.D., the Navari Family Professor of Life Sciences at Notre Dame, wrote, "His service to the profession, his membership on a number of editorial advisory boards and grant review panels and popularity as a consultant worldwide, and his reputation for superb training and placement of lab workers has been remarkable. His chemistry is noted for being innovative, yet practical and reproducible."

Mobashery's sentiments were echoed by John Macor, Ph.D., executive director of immunoscience discovery chemistry, Bristol Myers Squibb, who wrote about Miller, "His commitment to both research in organic and medicinal chemistry, coupled with his devotion to training the next generation of organic and medicinal chemists, makes him the ideal candidate for the MEDI Hall of Fame."

Professor Miller joined the College of Science in 1977 after earning a Ph.D. in bioorganic chemistry from Cornell University and following postdoctoral work at the University of California, Berkeley. In 1996, Miller was named the George & Winifred Clark Professor of Chemistry and Biochemistry at the University of Notre Dame.

Befittingly, two of Miller's former students have also been inducted into MEDI Hall of Fame: Macor was previously inducted in 2014, and Ann Weber was inducted along with Miller in 2016, a testament not only to Miller's own contributions to chemistry, but the lasting impact he has made on subsequent generations of chemists as well. ■

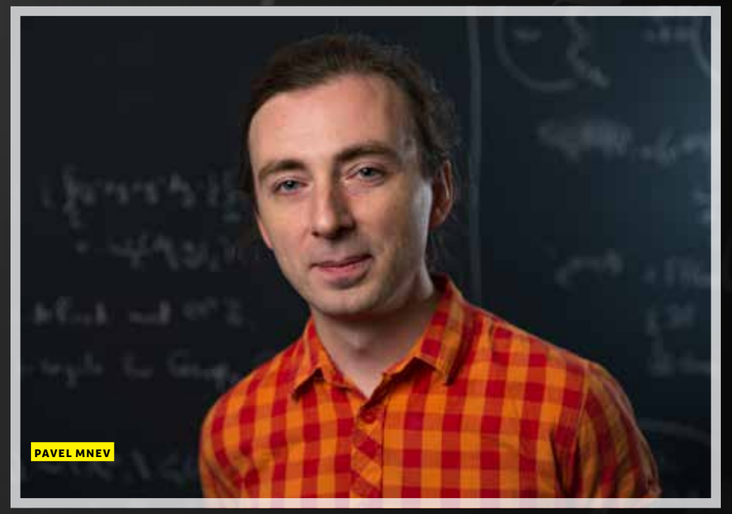
Notre Dame topologist awarded The André Lichnerowicz Prize in Poisson geometry

By Tammi Freehling

PAVEL MNEV, A NEW TOPOLOGIST AT THE College of Science in the Department of Mathematics, has been awarded The André Lichnerowicz Prize in Poisson geometry. The biennial award is given for outstanding work by a young mathematician in Poisson geometry. "I am very much honored by the award. It is most encouraging to be recognized by such a respected international research society," Mnev said. The André Lichnerowicz Prize is named in memory of André Lichnerowicz (1915–1998), whose work was fundamental in establishing Poisson geometry as a branch of mathematics.

Professor Misha Gekhtman described Poisson geometry as an area of mathematics that provides a geometric framework for investigation of intrinsic properties of classical and quantum physical systems. It both draws on techniques from, and influences a variety of, mathematical subjects, from analysis to algebra to topology. Mnev's work is at the interface of Poisson geometry, topology and mathematical physics. Professor Mark Behrens added that Mnev's work, "is based on the idea that if you know the local values of integrals over different regions of the space in which you are doing physics, you can get global expectation values over the whole space by a patching technique. Interestingly, he finds that you can read off certain topological invariants of the space you are doing physics on from these global expectation values."

Mnev, an assistant professor in the Department of Mathematics, received his Ph.D. in 2008 from the St. Petersburg Department of the Steklov Mathematical Institute of the Russian Academy of Sciences under the direction of Ludwig Faddeev, a group that is credited with a number of crucial developments in modern theoretical and mathematical physics. Mnev held a postdoctoral position at the University of Zurich and was most recently an advanced researcher at the Max Planck Institute for Mathematics in Bonn, home of the world's preeminent group working on applications of topology to physics. Mnev has been favorably compared to several senior researchers at top institutions, and brings much-desired expertise to the Department of Mathematics. ■



PAVEL MNEV

Understanding the rhythms of life

By Brian Wallheimer

OUT OF WHACK CIRCADIAN RHYTHMS CAN cause problems, from annoying jet lag to disastrous workplace accidents, to physical and mental illnesses.

Giles Duffield, associate professor, explores the genetic mechanisms that control our internal clocks. His work has led to discoveries of genes and molecular pathways that reset our circadian clocks and the mechanisms to more quickly reset those clocks.

The human body runs on a 24-hour cycle. That cycle is disrupted by a long trip through several time zones or changes in the sleep cycle, such as when a worker's hours regularly change. Shift workers, Duffield said, have higher instances of diabetes, metabolic syndrome, obesity, and certain types of cancer.

"Our body's metabolism changes on a 24-hour basis. During the day, we eat food and store energy molecules, and at night, we do the opposite—the energy molecules stored get released into the bloodstream and are used by the body," Duffield said. "But when we throw off that rhythm, which we tend to do more over the last century, we see these negative impacts. If we can find ways and means of manipulating the circadian clock, we can maybe change our physiology to deal with the demands of our society today."

Duffield's research identified the transcription factor gene ID2 as a significant player in resetting the circadian clock and controlling outputs associated with the clock, such as the time-of-day specific regulation of glucose and fat metabolism. Mice with a repressed ID2 gene showed profound changes in their behavior and physiology, such as an altered daily rhythm of physical activity and of feeding, reduced body fat deposits, a lower body temperature, and changes in their sensitivity to insulin and glucose.

Another gene, SIK1, which encodes a kinase enzyme, has been shown to affect the efficiency of the clock's reset mechanism. Generally, a circadian clock can be adjusted up to two hours in a day—which explains why someone traveling through 12 time zones may take six or more days to adjust.

Duffield found that inhibiting SIK1 at about the same time a subject is exposed to light—a key to resetting the circadian clock—can double that adjustment to four hours.

"One could imagine that you could design a drug that, when taken at the time you expose yourself to light, would relieve jet lag or help reset the clock when changing work shifts," Duffield said.

Duffield's work will continue to look at a mouse model of the fatty liver disease produced by chronic alcohol consumption that also shows disturbances to the rhythms of circadian clock genes. He's also interested in the rhythms that change in mosquitoes, including those controlling olfaction and insecticidal detoxification, causing them to be more aggressive feeders in the evening and more sensitive to the insecticide DDT in the morning. ■

GILES DUFFIELD explores the genetics behind our internal clocks.

Standing Ovations

Faculty Accolades

Twenty University of Notre Dame faculty members have received Rev. Edmund P. Joyce, C.S.C., Awards for Excellence in Undergraduate Teaching, including five science faculty: XAVIER CREARY, MORTEN ESKILDSEN, AMANDA HUMMON, SHAUN LEE, and JENNIFER ROBICHAUD.

PRASHANT KAMAT, the Rev. John A. Zahm Professor of Science in the Department of Chemistry and Biochemistry and Radiation Laboratory, was chosen to serve as the inaugural editor-in-chief of *ACS Energy Letters*.

JONATHAN HAUENSTEIN, an associate professor in the Department of Applied and Computational Mathematics and Statistics, received the Young Investigator Program Award from the Air Force Office of Scientific Research and the Office of Naval Research.

CLAUDIU RAICU, an assistant professor of mathematics, received an Alfred P. Sloan Research Fellowship.

Professors MARGARET DOBROWOLSKA, JACEK FURDYNA and XINYU LIU of the Department of Physics were recognized by the National Science Foundation with a Creativity Extension Award of $344,000.

DEE ANNE GOODENOUGH-LASHUA, associate professional specialist and academic advisor for biochemistry majors, received the Dockweiler Award, which recognizes faculty or staff members who have demonstrated a sustained commitment to Notre Dame undergraduates.

NANCY MICHAEL, an assistant teaching professor and director of undergraduate studies for neuroscience and behavior, received the Ganey Community Engagement Award for Research and Teaching.

Professors HAIFENG GAO and VLAD ILUC received the Early Career Development (CAREER) Award from the National Science Foundation.

JENNIFER TANK, the Galla Professor of Biological Sciences, received the 2016 Rodney F. Ganey, Ph.D., Community-Based Research Award for working with Kosciusko County farmers and local conservation staff to reduce nutrient runoff in the Shatto Ditch Watershed.

DAVID GALVIN, associate professor of mathematics, received the 2016 Father James L. Shilts, C.S.C./Doris and Gene Leonard Teaching Award from the College of Science.

MARVIN MILLER, professor emeritus of chemistry, was selected for induction into the American Chemical Society Division of Medicinal Chemistry Hall of Fame.

STEVEN CORCELLI, associate professor of chemistry and biochemistry, was selected as a member of the 2016 Fellows of the American Chemical Society.

PAVEL MNEV, a new topologist at the College of Science in the Department of Mathematics, was awarded the André Lichnerowicz Prize in Poisson geometry.

FRANÇOIS LEDRAPPIER, professor emeritus of mathematics, directeur de recherche with the French CNRS, and member of the Probability and Random Models Laboratory at the Université Paris VI, was awarded a Grand Prize of the French Academy of Sciences.

ANI APRAHAMIAN, Freimann Professor of Physics was named co-chair of a committee with the National Academy of Science on a U.S. Electron Ion Collider Facility.

Notre Dame chair in astrophysics, TIMOTHY BEERS, and nuclear astrophysicist REBECCA SURMAN, were elected Fellows of the American Physical Society (APS) by the APS Council of Representatives at its September 2016 meeting.

DONALD LINCOLN, a guest professor in physics, has been named a Fellow of the American Association for the Advancement of Science.

SERGEI STARCHENKO, professor of mathematics, was named a fellow in the American Mathematical Society.

CODY J. SMITH, the Elizabeth and Michael Gallagher Assistant Professor of Neural Development and Regeneration, has been selected as a recipient of the prestigious Sloan Research Fellowship.

ALEX PERKINS, Eck Family Assistant Professor, and member of the Department of Biological Sciences, the Department of Applied and Computational Mathematics and Statistics, the Eck Institute for Global Health, and the Environmental Change Initiative, was named an Early Career Fellow by the Ecological Society of America.

PAUL W. BOHN, the Arthur J. Schmitt Professor of Chemical and Biomolecular Engineering and concurrent professor of chemistry and biochemistry, has been appointed to the editorship of *Annual Reviews of Analytical Chemistry*.

PETER C. BURNS, concurrent professor of chemistry and biochemistry, was honored by the Mineralogy Association of Canada at their annual meeting with the 2016 Peacock Medal.

Alumnus Spotlight

John G. Meara

Surgeon-in-Chief opens doors for global surgical accessibility

By Shadia Ajam

IN SPRING 2016, ALUMNUS JOHN G. MEARA M.D., DMD, MBA, (ND '86) delivered a presentation at Notre Dame on safe surgical care worldwide. Meara is currently the Plastic Surgeon-in-Chief of the Boston Children's Hospital. He is also associate professor of surgery and associate professor of global health and social medicine at Harvard Medical School.

Meara focused on explaining the mission of the Lancet Commission on Global Surgery, where he serves as a co-chair. The commission consists of professionals from diverse backgrounds who strive to develop and assemble the best evidence on the state of surgery worldwide, to study the economics of surgical and anesthesia care delivery, and to develop strategies for improving access.

On April 27, 2015, the Lancet Commission's findings were published in a report, launched in London at the Royal Society of Medicine. The report, titled "Global Surgery 2030: evidence and solutions for achieving health, welfare, and economic development", contained five key messages for health policy makers:

1. Five billion people lack access to safe, affordable surgical and anesthesia care when needed.
2. One hundred forty-three million additional surgical procedures are needed each year to save lives and prevent disability.
3. Thirty-three million individuals face catastrophic health expenditure due to payment for surgery and anesthesia each year.
4. Investment in surgical and anesthesia services is affordable, saves lives, and promotes economic growth.
5. Surgery is an indivisible, indispensable part of health care.

The commission's findings have been implemented in Cabo Verde, Zambia, Madagascar, and India. In Zambia, the Commission partnered with the ministry of health to design and implement a contextually-tailored National Surgical and Anesthesia Plan based off the framework developed by the commission.

Meara said to undergraduate students, "When I think about where you guys are; you're going to start to make some more career-based decisions. Over the next 10 years, you're going to start to weave a vocational career. You're going to be leading non-governmental organizations in the future—don't underestimate what you're capable of doing. Coming from Notre Dame is hugely beneficial."

To learn more about the Lancet Commission on Global Surgery visit lancetglobalsurgery.org/

Flipping the classroom

By Gene Stowe

AN EXPERIMENT WITH FLIPPED CLASSROOMS—VIDEO LECTURE VIEWING for homework and group problem-solving in class–in lower-level mathematics classes has heightened student engagement and learning. Enabled by new technologies, including a Lightboard that facilitates recording lectures, the strategy makes teachers' expertise available to students when they need it most. Group work ensures positive peer pressure to complete before-class assignments, builds knowledge as they teach each other, and develops leadership.

Anne Bernadette Pilkington, an associate professional specialist in mathematics, organized the structure after she heard of the benefits of flipped classrooms. Graduate students Brian Stoyell-Mulholland and P.J. Jedlovec also use the method. Juniors and seniors assist with the problem sessions. The approach has been used in Principles of Calculus, Principles of Finite Mathematics, Calculus 2, and Calculus 3. A Teaching Innovation Grant from the College of Science has helped support the work.

"It feels more like teaching to me than standing in a lecture hall pontificating," Pilkington said. "I got to know the students much better. The idea was that students would work in a group and one would present at a whiteboard and work a problem. They could discuss it and argue about it. We would circulate and be able to answer questions as they arose instead of just standing there and lecturing."

Stoyell-Mulholland, a fourth-year Ph.D. candidate who expects to focus on mathematics education in his career, has taught four classes with flipped classrooms and believes students typically pay more attention in the problem-solving classes than lectures. "Besides the mathematics that developed, a side bonus I saw was student leadership," he said. "They found that they were able to teach each other the material and look to me for verification and some directional support."

Jedlovec, a fourth-year Ph.D. candidate who has been teaching for three years, said the method is especially appropriate for mathematics. "What is most helpful is to have an expert in the field there with you to help you solve problems, to do the really difficult part," he said.

Mathematics Department Chair Jeffrey Diller said the initiative demonstrates the benefits of graduate students teaching undergraduates, not least because they have recent memory of what it was like to struggle with the material. "Graduate students bring to the classroom youth, energy, and an openness to new things. They take it very seriously and have a lot of good ideas." ■

ANNE BERNADETTE PILKINGTON demonstrates the Lightboard technology that makes flipped classrooms possible.

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The University of Notre Dame Environmental Research Center, UNDERC, provides world-class destinations for environmental research, unsurpassed undergraduate education programs, and innovative graduate student training in Montana (shown here) and in the Upper Peninsula of Michigan.

Photo by Barbara Johnston