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Arkansas Catalyst, February 2013

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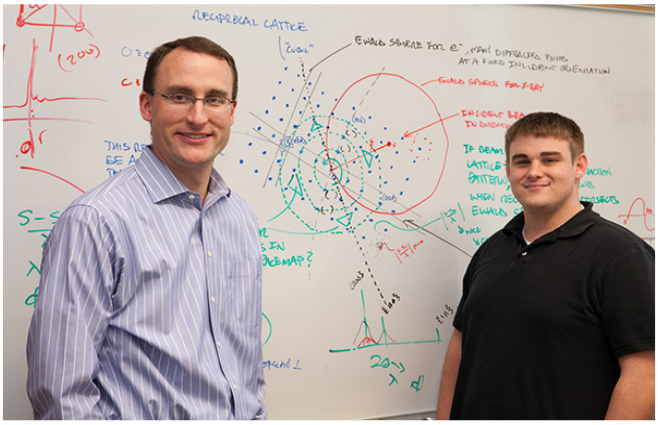
The Arkansas Catalyst

February 2013

Supercomputing Network Awards Grants to Researchers



Doug Spearot (left), associate professor of mechanical engineering, and doctoral student Shawn Coleman.

Douglas Spearot, an associate professor of mechanical engineering, and doctoral student Shawn Coleman are working to solve a computational problem in nanoscale material behavior. They are conducting research with the aid of supercomputers located in San Diego and Austin, Texas.

Their project was among three major awards of supercomputer time recently allocated to U of A researchers by the Extreme Science and Engineering Discovery Environment, a collection of facilities that scientists can use to interactively share computing resources, data and expertise.

The awards to the university total 3.6 million "service units" on supercomputers at sites ranging from California to Tennessee. The units, equivalent to core computing hours, are worth approximately $288,000 based on estimates by the National Science Foundation and XSEDE, according to Jeff Pummill, manager of cyberinfrastructure enablement at the university's Arkansas High Performance Computing Center. The center helped prepare the supercomputer time-grant proposals.

In addition to Spearot and Coleman, Douglas Rhoads, professor of biological sciences, and Xuan Shi, an assistant professor of geosciences, received awards of supercomputer time. Shi was awarded time at supercomputers at the National Institute for Computational Sciences in Oak Ridge, Tenn., to accelerate computations centering on crime data and urban sprawl simulations. Rhoads is working with Pummill on assembling the complete genome for the timber rattlesnake. A better understanding of the reptile genome has implications for human health, among other things. They were awarded time on supercomputers in San Diego, Austin and Pittsburgh.

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Chemist Receives NSF Early Career Award

Colin Heyes, left, and research collaborator Nela Durisic.

Colin Heyes, an assistant professor in the department of chemistry and biochemistry in the J. William Fulbright College of Arts & Sciences at the University of Arkansas, has received a $650,000 Faculty Early Career Development Program award from the National Science Foundation.

The award was given to further his investigation of the interfaces between the core and shell of colloidal quantum dots.

Colloidal quantum dots are microscopic semiconductor crystals that are grown in solution. Adding a shell to the core quantum dot provides a way to control the functionality of these crystals, which can be used to emit light for biomedical imaging, LEDs and spectroscopy or photocurrents for solar cells and chemical sensors. The research will help scientists better understand the relationship between the structure of the quantum dot and its functionality.

"All of these modern applications rely on the same fundamental electronic processes within quantum dots," Heyes said. "Our work will provide a better understanding of how to control these crystals to eventually build brighter, faster, longer-lasting and more efficient products."

The grant will support Heyes' research in this area for the next five years and will encourage and promote the

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IN OTHER NEWS

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Sign up for Listserv information on the six interdisciplinary research strengths at the University of Arkansas: health, energy and environment, nanoscience and engineering, supply chain logistics and transportation, food safety, and American art, architecture and the humanities.

AWARD WINNERS

The following is a sampling of faculty awards in February, with the principal investigator, the award amount and the sponsor. An asterisk (*) indicates the continuation of a previous

participation of graduate, undergraduate and minority students. As part of the grant, a two-week, hands-on workshop will be held each summer on the U of A campus.

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Blair-Clinton School Poll Provides National Public Opinion

Americans believe higher education institutions and the federal government share almost equal responsibility for student loan debt in the country. This is one preliminary result from a comprehensive national research survey sponsored by two entities of the University of Arkansas System.

The nonpartisan academic poll was conducted by the Diane D. Blair Center of Southern Politics and Society at the University of Arkansas in Fayetteville and the University of Arkansas Clinton School of Public Service in Little Rock. An early look at the results shows public opinion regarding issues such as student loan debt, the killing of Osama bin Laden and the 2012 presidential election.

This is the Blair Center's second election year to administer the national poll and the first time it was conducted in partnership with the Clinton School. The project was founded by an interdisciplinary group of scholars from the Blair Center including Todd Shields, Angie Maxwell, Pearl Ford Dowe and Rafael Jimeno.

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Faculty, Students Solve Biochemistry Problem

Denise Greathouse, University of Arkansas

After years of experimentation, researchers at the University of Arkansas have solved a complex, decades-old problem in membrane biochemistry.

The consequence of their work will give scientists more information about the function and structure of proteins.

award.

- Sean Mulvenon, $3,098,365, The Corporation for Developing Awareness of World Need Inc.
- Denise Airola, $194,300, Arkansas Department of Education
- Jackson Cothren, $30,074, Endeavor Foundation
- Feng Wang, $24,602, National Science Foundation
- Tyrone Washington, $20,000, University of Arkansas for Medical Sciences

"Historically, lysine and arginine, both basic amino acids, were considered to have very similar properties and therefore to be essentially interchangeable," said Denise Greathouse, a research associate professor in the department of chemistry and biochemistry. "Our results demonstrate that despite their similarities, the differences in their behavior in membrane environments provide important clues for understanding membrane protein function."

The findings appeared in the January issue of the journal Proceedings of the National Academy of Sciences. Greathouse, former doctoral students Nicholas Gleason and Vitaly Vostrikov, and Roger Koeppe II, Distinguished Professor of chemistry and biochemistry, wrote the article, "Buried lysine, but not arginine, titrates and alters transmembrane helix tilt."

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CONTACT US

Vice Provost for Research and Economic Development
205 Administration Building
1 University of Arkansas
Fayetteville, AR 72701
479-575-2470

email us

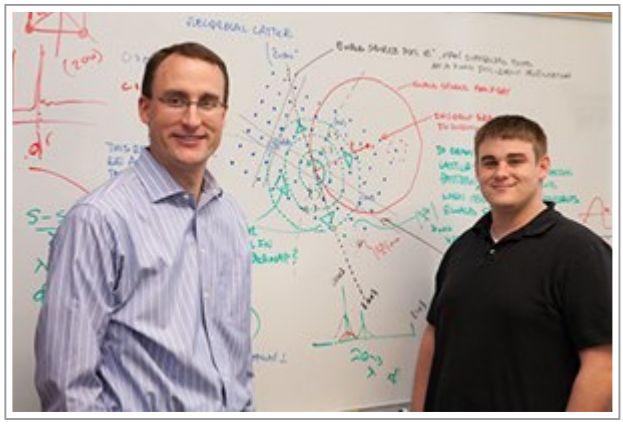
University of Arkansas Arkansas Newswire

National Supercomputing Network Awards Grants to University of Arkansas Researchers

Three projects allocated time worth an estimated $288,000

Monday, February 04, 2013

FAYETTEVILLE, Ark. – The white board in Douglas Spearot's office in the Institute for Nanoscience and Engineering at the University of Arkansas is a symphony of green, red and black drawings and equations.



Doug Spearot (left), associate professor of mechanical engineering, and doctoral student Shawn Coleman received an award of supercomputer time through the Extreme Science and Engineering Discovery Environment. Photo by Russell Cothren, University of Arkansas.

Spearot, an associate professor of mechanical engineering, and doctoral student Shawn Coleman are working to solve a computational problem in nanoscale material behavior. The work on the white board represents research they are conducting with the aid of supercomputers located in San Diego and Austin, Texas.

Their project was among three major awards of supercomputer time recently allocated to U of A researchers by the Extreme Science and Engineering Discovery Environment, a collection of facilities that scientists can use to interactively share computing resources, data and expertise. The collected facilities, known as XSEDE, are supported by the National Science Foundation and offer researchers access to a network of 16 supercomputers and high-end visualization and data analysis resources across the United States.

The awards to the U of A total 3.6 million "service units" on supercomputers at sites ranging from California to Tennessee. The units, equivalent to core computing

hours, are worth approximately $288,000 based on estimates by the National Science Foundation and XSEDE, according to Jeff Pummill, manager of cyberinfrastructure enablement at the university's Arkansas High Performance Computing Center. A core hour is the amount of work that would be done by just one central processing unit core in one hour's time.

The researchers don't travel to the supercomputer sites; they connect to the supercomputers from their campuses and remotely submit jobs that often require hundreds of processors and hundreds of terabytes of memory. A terabyte is equal to 1 trillion bytes, or 1,000 gigabytes.

XSEDE, formerly known as TeraGrid, awarded several smaller supercomputing resource grants in the last three years to the U of A. The recent awards are the most substantial, Pummill said.

Rick McMullen, director of the Arkansas High Performance Computing Center, said the center's mission is to meet the computational needs of the U of A community, either on campus or with supercomputers at other sites.

"The National Science Foundation has a meticulous process of peer-review for this type of XSEDE award, so it's significant to get this kind of time," McMullen said.

In addition to Spearot and Coleman, Douglas Rhoads, professor of biological sciences, and Xuan Shi, an assistant professor of geosciences, received awards of supercomputer time.

Spearot said calculations performed at the high performance computing center provided feasibility results that strengthened the proposal he and Coleman submitted to XSEDE. Coleman is attending the university on a Doctoral Academy Fellowship.

"The computer time awarded will allow Shawn to perform atomistic simulations critical to his dissertation that are too computational and memory-intensive to be performed on local resources," Spearot said.

Shi was awarded time at supercomputers at the National Institute for Computational Sciences in Oak Ridge, Tenn., to accelerate computations centering on crime data and urban sprawl simulations.

Rhoads is working with Pummill on assembling the complete genome for the timber rattlesnake. A better understanding of the reptile genome has implications

for human health, among other things. They were awarded time on supercomputers in San Diego, Austin and Pittsburgh.

The Arkansas High Performance Computing Center helped prepare the supercomputer time-grant proposals.

Contacts:

Rick McMullen, director
Arkansas High Performance Computing Center
479-575-8681, dfmcmull@uark.edu (mailto:dfmcmull@uark.edu)

Douglas Spearot, associate professor and 21st Century Professor
College of Engineering
479-575-3040, dspearot@uark.edu (mailto:dspearot@uark.edu)

Chris Branam, research communications writer/editor
University of Relations
479-575-4737, cwbranam@uark.edu (mailto:cwbranam@uark.edu)

University of Arkansas Arkansas Newswire

Chemist Receives National Science Foundation Early Career Award

Heyes studies the interface between core and shell of quantum dots

Tuesday, February 05, 2013

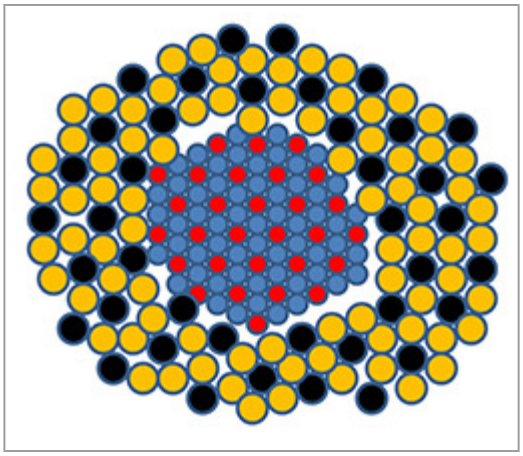
FAYETTEVILLE, Ark. – Colin Heyes, an assistant professor in the department of chemistry and biochemistry in the J. William Fulbright College of Arts & Sciences at the University of Arkansas, has received a $650,000 Faculty Early Career Development Program award from the National Science Foundation. The award was given to further his investigation of the interfaces between the core and shell of colloidal quantum dots.

Colin Heyes, left, and research collaborator Nela Durisic align the optical components of a microscope to improve its sensitivity to detect single quantum dots.

Colloidal quantum dots are microscopic semiconductor crystals that are grown in solution. Adding a shell to the core quantum dot provides a way to control the functionality of these crystals, which can be used to emit light for biomedical imaging, LEDs and spectroscopy or photocurrents for solar cells and chemical sensors. The research will help scientists better understand the relationship between the structure of the quantum dot and its functionality.

“All of these modern applications rely on the same fundamental electronic processes within quantum dots,” Heyes said. “Our work will provide a better understanding of how to control these crystals to eventually build brighter, faster, longer-lasting and more efficient products.”

Heyes studies the interfacial chemistry between the core, shell and ligands of colloidal quantum dots. Ligands sit on the shell surface and “hold” the colloidal quantum dots in solution; they also provide a chemical connection to the “outside world” so that quantum dots can attach to biological cells, solar cells or act as chemical sensors.



There is a lack of fundamental understanding about the structural properties of the core-shell and shell-ligand interfaces. Scientists can observe the boundary between the core and shell materials using powerful electron microscopes, but they do not yet understand how the nature of the structural mismatches between the two materials affects their optical and electrical properties. These mismatches create “holes” or “trap states” that result in losing control of excitons, which are electrons that have been energetically excited. The inability to control excitons result in energy lost as heat rather than converted into useful energy, such as light or electrical currents.

The NSF grant will expand Heyes’ investigation of how the optical and electrical properties of quantum dots are related to the core-shell and shell-ligand interfaces at the single quantum dot level. Understanding single quantum dots is necessary to advance miniaturized optoelectronics and single molecule fluorescence applications. His research team has produced preliminary data demonstrating that as these interfaces are systematically varied, the optical properties of single quantum dots can be tuned.

“We hypothesize that understanding the relationship between the structures of the core-shell or shell-ligand interfaces and the trap states will allow us to more precisely control these excitons that underlie the optical and electrical properties,” Heyes said.

Heyes’ team will focus specifically on understanding how the trap states are formed and how they contribute to the optical and electronic properties with the eventual goal of avoiding their formation altogether.

The grant will support Heyes' research in this area for the next five years and will encourage and promote the participation of graduate, undergraduate and minority students. As part of the grant, a two-week, hands-on workshop will be held each summer on the U of A campus. Undergraduate students from the university and from undergraduate institutions in Arkansas and Oklahoma will perform research experiments in Heyes' lab to promote and foster their interest in chemistry and nanomaterial science for eventual careers in the fields of science, technology, engineering and math.

Contacts:

Colin Heyes, assistant professor, chemistry and biochemistry
J. William Fulbright College of Arts & Sciences
479-575-5607, cheyes@uark.edu (mailto:cheyes@uark.edu)

Matt McGowan, science and research communications officer
University Relations
479-575-4246, dmcgowa@uark.edu (mailto:dmcgowa@uark.edu)

University of Arkansas Arkansas Newswire

Blair Center-Clinton School Poll Gives Early Context for 2012 Presidential Election Results, Much More

Poll provides national public opinion on wide range of topics

Wednesday, January 23, 2013

FAYETTEVILLE, Ark. – Americans believe higher education institutions and the federal government share almost equal responsibility for student loan debt in the country. This is one preliminary result from a comprehensive national research survey sponsored by two entities of the University of Arkansas System.

Among demographic groups, white, African American and Latino/Latina American respondents largely blame colleges and universities (31 percent) and the federal government (30 percent) for the large amount of student debt, which reached nearly $1 trillion last year. Smaller percentages of these groups blame students (18 percent), state governments (7 percent) and parents (4 percent).

The nonpartisan academic poll was conducted by the Diane D. Blair Center of Southern Politics and Society at the University of Arkansas in Fayetteville and the University of Arkansas Clinton School of Public Service in Little Rock. An early look at the results shows public opinion regarding issues such as student loan debt, the killing of Osama bin Laden and the 2012 presidential election.

“In addition to in-depth findings about a wide array of topics, we wanted to sample issues that are relevant to some of the current political and public policy debates in the news today,” said Clinton School Dean Skip Rutherford. “The findings are very interesting and should add to the conversation about issues such as the growing student loan debt problem in our country.”

This is the Blair Center’s second election year to administer the national poll and the first time it was conducted in partnership with the Clinton School. The project was founded by an interdisciplinary group of scholars from the Blair Center including Todd Shields, Angie Maxwell, Pearl Ford Dowe and Rafael Jimeno.

“These questions are only a glimpse into the findings of this comprehensive survey,” said Shields, director of the Blair Center. “More in-depth findings will be released through a series of reports over the next several months, exploring in detail these issues as well others about immigration, community philanthropy, racial attitudes, religion and regional trends.”

Several questions focused on presidential politics, including views on the 2012 election. Roughly half of the respondents said they voted for President Barack Obama and 42 percent said they voted for Gov. Mitt Romney, while the remainder did not respond. Men were more likely to have voted for Romney (46 percent), while women were more likely to have supported the president’s reelection (56 percent).

Support for Romney was higher overall in the South than elsewhere, but results indicated significant racial and regional gaps.

Of the Southern respondents who reported to have voted in the election, 67 percent of whites, 2 percent of African Americans and 32 percent of Latinos indicated they voted for Romney, while 33 percent of whites, 98 percent of African Americans and 66 percent of Latinos in the South indicated they voted for Obama.

Of the respondents outside the South who reported to have voted in the election, 47 percent of whites, 2 percent of African Americans and 28 percent of Latinos indicated they voted for Romney, while 46 percent of whites, 95 percent of African Americans and 72 percent of Latinos outside the South indicated they voted for Obama.

When respondents were asked to assign a percentage of credit to various political actors in the May 1, 2011, raid that resulted in the killing of Osama bin Laden, the

largest share of the credit (44 percent) was given to the Navy Seal team that conducted the raid. President Obama was next (23 percent) followed by the U.S. intelligence agencies (22 percent), President George W. Bush (4 percent) and Secretary of State Hillary Clinton (3 percent). While whites gave the Navy Seal team almost 50 percent of the credit and only 18 percent to Obama, African Americans gave Obama 45 percent of the credit compared to 27 percent for the Navy Seals.

A question about Romney's Mormon faith drew varying responses among demographic groups. A roughly equal number of respondents believe that Romney is Christian (37 percent) as those who said they didn't know if he is a Christian (38 percent). More than half of those who identified themselves as Republicans said they believed Romney is a Christian while only 28 percent of Democrats and 26 percent of Independents did so.

The questions covered in this initial release of results account for only a small portion of the poll topics. Researchers with the Blair Center, Clinton School and other entities will use the data gathered in the full survey for a number of projects, including a series of reports on the 2012 presidential election that the Blair Center will release in the next few months.

"Because of the depth of this research, we will be able to analyze differences that emerge by gender, race, religion, political affiliation, socioeconomic status and the intersection of these characteristics," said Maxwell, an assistant professor of political science with the Blair Center."It will be invaluable for scholars, journalists and students."

The Blair Center-Clinton School Poll, completed in mid-December, surveyed more than 3,600 people regarding issues related to politics, giving, regional identification, religion, racial discrimination, ideology and partisanship. The poll has a margin of error of 2.5 percentage points.

The poll was administered by GfK, formerly Knowledge Networks, the leader in web-based survey research. GfK's proprietary database features a representative sample of Americans, including representation of the roughly 30 percent of U.S. households that do not have Internet access. The database covers the growing number of cell phone-only households, recently estimated at 23 percent of all households, through address-based sampling. The survey was conducted in both English and Spanish.

Though national in scope, the poll uniquely included representative samples of traditionally under-polled groups such as African Americans, Latinos and southern whites and measured their attitudes on a host of contemporary political and public policy issues. A full analysis of five newsworthy questions asked in the poll is attached.

Blair Center and Clinton School scholars will discuss the poll at a public program on Wednesday, Feb. 6, at the Clinton School. The program will mark the release of another report from the poll data on "The Year of the Woman," in which scholars analyze views on women's issues and women in politics.

See the full report of the Blair Center-Clinton School (http://blaircenterclintonschoolpoll.uark.edu/6715.php) survey. For more information about the Blair Center-Clinton School partnership, please visit blaircenterclintonschoolpoll.uark.edu (http://blaircenterclintonschoolpoll.uark.edu/) or bccs.uark.edu (http://bccs.uark.edu/) .

About the Partners:

The Diane D. Blair Center of Southern Politics and Society, part of the J. William Fulbright College of Arts and Sciences at the University of Arkansas, was established in 2001 by an act of the U.S. Congress. This research center was named in honor of Diane Divers Blair who taught in the Political Science Department at the University of Arkansas for 30 years. The Blair Center reflects her academic model and strives to approach the study of the American South from a variety of angles, attempting to reveal the undercurrents of politics, history and culture that have shaped the region.

The nation's seventh presidential school, the University of Arkansas Clinton School of Public Service is the first school in the nation to offer a Master of Public Service (M.P.S.) degree, giving students the knowledge and experience to further their careers in the areas of nonprofit, governmental, volunteer or private sector service. Additionally, the mission of the Clinton School's Center on Community Philanthropy, directed by Charlotte Williams, is to promote issues and research into community-based philanthropy and its role in generating social, economic and political change.

Contacts:

Ben Beaumont, director of communications
University of Arkansas Clinton School of Public Se
501-454-2779, bbeaumont@clintonschool.uasys.edu
(mailto:bbeaumont@clintonschool.uasys.edu)

Darinda Sharp, director of communications
J. William Fulbright College of Arts and Sciences
479-575-3712, dsharp@uark.edu (mailto:dsharp@uark.edu)

University of Arkansas Arkansas Newswire

Researchers Solve Complex Problem in Membrane Biochemistry Through Study of Amino Acids

New method opens door for better understanding of protein function

Thursday, January 24, 2013

Denise Greathouse and Roger Koeppe II

FAYETTEVILLE, Ark. – After years of experimentation, researchers at the University of Arkansas have solved a complex, decades-old problem in membrane biochemistry. The consequence of their work will give scientists more information about the function and structure of proteins, the workhorses within the cells of the human body.

“Historically, lysine and arginine, both basic amino acids, were considered to have very similar properties and therefore to be essentially interchangeable,” said Denise Greathouse, a research associate professor in the department of chemistry and biochemistry. “Our results demonstrate that despite their similarities, the differences in their behavior in membrane environments provide important clues for understanding membrane protein function.”

The findings, which appear in the January issue of the journal *Proceedings of the National Academy of Sciences*, address long-standing questions in the study of protein structure and function and help explain how charged amino acids are able to modulate the behavior of proteins in cellular membranes.

Greathouse, former doctoral students Nicholas Gleason and Vitaly Vostrikov, and Roger Koeppe II, Distinguished Professor of chemistry and biochemistry, wrote the

article, “Buried lysine, but not arginine, titrates and alters transmembrane helix tilt.”

Proteins do nearly all the work in the cells of our bodies, ranging from brain function and nerve transmission to metabolic energy production and muscular contraction. Moreover, many diseases are associated with defects in protein function. Future advances in the diagnosis and treatment of human disease will depend upon better understanding of the thousands of proteins that are encoded within the genomes of humans and human pathogens.

The structure and function of membrane proteins both play a crucial role in cell signaling and the regulation of biological function. The authors developed experimental methods that determine how lysine and arginine interact in the lipid bilayer membrane environment. In the last 10 years there have been computational predictions of the behavior of lysine and arginine in the membrane but not methods to test those predictions.

“It is the first measurement of its type, its complexity makes it an elegant method, and it opens the door for other people to apply these methods on biologically important problems,” Koeppe said. “There is a lot of interest in trying to understand what’s going on in these membranes, especially with protein molecules that carry particular electric charges. Unless we can understand it at the fundamental level, then we can’t extrapolate it to the nervous system. We’re trying to develop foundational knowledge that is needed to understand the nervous system.

“We’re excited about this study because it makes available knowledge that other researchers can use,” he said. “Those making the computer predictions can refine their methods and make better predictions because they know that they were able to reproduce some of our results.”

Lysine and arginine are ionizable, which means they can have a positive electric charge. The research team created a framework for experimentation that uses magnetic resonance imaging to measure whether the groups remain charged or become uncharged as the acidity or the pH of the environment is changed. To make their procedure work, the scientists synthesized peptides, which are chemical compounds consisting of several or more linked amino acids. To enable the magnetic resonance experiments, some of the hydrogen atoms in the peptides were replaced with deuterium, a heavy isotope of hydrogen.

“We’ve spent about 15 years doing this,” Koeppe said. “We developed first- and second-generation families of model peptides, and we examine them in model lipid membranes in order to understand the properties of real cell membranes and real cell proteins. This is at a molecular level. We are not even up to the cell yet.”

Vostrikov and Gleason earned their doctorates in 2011 and 2012, respectively. Vostrikov is a postdoctoral fellow at the University of Minnesota and Gleason teaches chemistry at Shiloh Christian School in Springdale.

The National Science Foundation provided the grant for the experiments described in the *Proceedings of the National Academy of Sciences*. The National Institutes of Health provided the financial support for the early stages of development of the peptide framework and for the facilities.

The research was performed in the U of A’s Center for Protein Structure and Function, which was established in 2000 in the J. William Fulbright College of Arts and Sciences to develop a detailed understanding of the structure and function of proteins that could lead to improved treatments of human disease. Center scientists study proteins involved in cancer, heart disease, osteoporosis, the flu and other diseases and conditions.

Contacts:

Roger Koeppe II, Distinguished Professor, chemistry and biochemistr
J. William Fulbright College of Arts and Sciences
479-575-4976, rk2@uark.edu (mailto:rk2@uark.edu)

Chris Branam, research communications writer/editor
University Relations
479-575-4737, cwbranam@uark.edu (mailto:cwbranam@uark.edu)