UNIVERSITY OF ARKANSAS
J. WILLIAM FULBRIGHT COLLEGE OF ARTS & SCIENCES

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Department of Chemistry and Biochemistry

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Special points of interest:

- Koeppe lab publishes new insights for membrane proteins
- Protein Data Bank submission
- Meet the new graduate students
- NSF Career Award

Inside this issue:

New Labs for the New Year

All four organic labs on the first floor of SCIE were completely demolished and remodeled. New benches, drawers, hoods, and whiteboards were installed, replacing some very outdated equipment. It took eight days to clear out the old labs before construction could start. The job began on the Monday before Thanksgiving and finished on the Sunday night before classes began on January 14, 2013.

The new arrangement utilizes 8 hoods per lab. We can now run a single section in one lab for 16 students (8 hoods x 2 =16). This means that we can run 4 lab sections at the same time, now accommodating a maximum of 64 students, which computes to a net gain of 24 students per lab time. An immediate payback here includes the elimination of Sunday and Friday night labs.

Of the 100 lab sections offered this semester, 47 of them utilize the first floor lab spaces. They are also being utilized to accommodate 10 sections of the new 1131L (lab for engineers).

On the Go

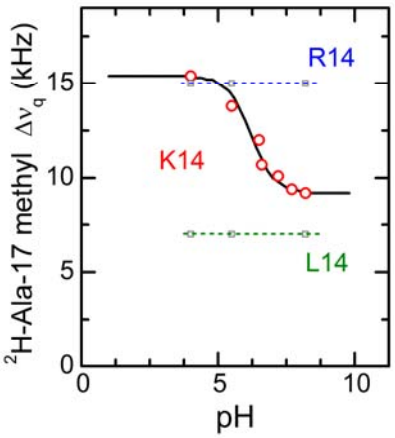
Ingrid Fritsch, "Redox-Magnetohydrodynamic (MHD) Microfluidics: Advantages and Challenges," Society of Western Analytical Professors (SWAP) Meeting, Fort Collins, CO, January 18-19, 2013.

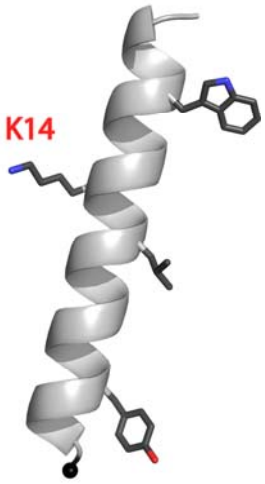
Publications

The article (**Philominathan, Koide, Matsushita and Sakon**, "Bacterial collagen-binding domain targets under-twisted regions of collagen," *Protein Science*, 2012) has been recommended as being of special significance in its field by "F1000 Faculty."

Titrations in Lipid Membranes

New insights for membrane proteins were published by **Nick Gleason** (Ph. D., 2012), **Vitaly Vostrikov** (Ph. D. 2011), **Denise Greathouse** and **Roger Koeppe**, in the January 2013 *Proceedings of the National Academy of Sciences*. The article, "Buried lysine, but not arginine, titrates and alters transmembrane helix tilt," addresses long-standing questions in membrane biochemistry and helps explain how charged amino acids modulate the behavior of proteins in cellular membranes.





Charged groups on membrane proteins play crucial roles in cell signaling, yet a key unresolved question is: Which groups are actually charged in the cell membrane environment at physiological pH? The authors developed experimental methods for indirect measurements of the ionization behavior of lysine and arginine in a membrane environment. Their results indicate that arginine in a lipid bilayer is fully charged at physiological pH, but lysine under the same conditions is charged only to an extent of 50% or less.

Over the past 15 years the Koeppe research group has developed first– and second-generation families of model peptides and examined them in lipid membranes. Their latest peptide framework incorporates specific deuterium atoms, as probes for solid-state NMR spectroscopy, and serves as a "host" system for individual "guest" residues (such as lysine or arginine). The deuterium NMR spectra report the orientation and dynamics of a peptide helix, which in turn report whether a guest residue remains charged, or becomes uncharged, as the pH of the environment is changed. In the last 10 years there have been computational predictions of the behavior of lysine and arginine membranes but not methods to test those predictions. The new experiments open the door for refinement and validation of computational methods and for subsequent investigations of biologically important problems.

Financial support was provided by the National Science Foundation, the NIH COBRE Center for Protein Structure and Function, and the Arkansas Biosciences Institute. Additional information is available at http://newswire.uark.edu/article.aspx?id=20029.

Protein Data Bank Submissions

The Protein Data Bank (PDB) archive is the single worldwide repository of information about the 3D structures of large biological molecules, including proteins and nucleic acids. The following coordinates were submitted to the Protein Data Bank by undergraduate students (**E Gill, JR Rosser, JM Sanders**) in 2012; 4G57, 4H7B, and 41D6. The coordinates were verified and released in 2012. Two other sets of coordinates submitted by an undergraduate student (**D Weir**) are in verification process by PDB editors. Coordinates submitted by graduate student **R Bauer**, 4HPK and 3JQW, are now verified and should be released shortly!

New Graduate Students

Kaiyang Leong, Singapore, received his BA in Chemistry from Boston University.

Nandita Halder, India, received her B.Sc.Engg. (MME) degree from Bangladesh Univ. of Engineering, Dhaka. No photo of Nandita was available at press time.

Heyes Receives NSF Career Award

Colin Heyes, assistant professor in the department of chemistry and biochemistry, has received a Faculty Early Career Development (CAREER) Program award from the National Science Foundation for his investigation of the interfaces between the core and shell of colloidal quantum dots. The $650,000 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.

A major leap forward in the development of quantum dots was enabled by the discovery that a shell could be grown on the core semiconductor material. This core-shell configuration allows opportunities to control the movement of excitons to produce either light emission or electrical current. Today, these materials have current applications in biomedicine, renewable energy and biological and chemical sensors. Improved understanding and manipulation of quantum dots will aid in the future development of ultrasensitive medical diagnostics, tunable lasers, LED lighting, optical storage and even quantum computing.

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." Currently, 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 lattice mismatches between the two materials affects their optical and electrical properties. Theses mismatches create "holes" or "trap states" that result in losing control of the excitons, and their energy is lost as heat rather than producing light or electrical currents. Additional trap states can be produced at the shell-ligand interface, but these are much more difficult to observe and must be done spectroscopically.

The grant will further Heyes' investigation of how the optical and electrical properties are related to the core-shell and shell-ligand interfaces at the single quantum dot level, which is necessary for 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 and tuning the core-shell interface will provide us with more precise control of the excitons that underlie the coupled 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 excited electronic energy. They will do this by 1) synthesizing a range of core-shell and core multi-shell material configurations and structurally characterizing these interfaces using high-resolution electron microscopy available at the new Institute for Nanoscience and Engineering, 2) analyzing the influence of the core-shell interfaces on optical and electronic properties, and 3) evaluating how these properties depend on the shell-ligand interface and the external environment. "The ability of quantum dots to produce photon emission for spectroscopy, imaging and LEDs or to produce photocurrents for solar cells and chemical sensors are all controlled by the same fundamental electronic processes," Heyes said. "Electron-hole recombination to produce light and charge-carrier transfer across quantum dot interfaces to produce electrical current compete with each other, and the winner will control their final application. Our work will provide a better understanding of how to control them."

As part of the grant, a two-week, hands-on workshop will be held each summer. Undergraduate students from the university and from undergraduate institutions in Arkansas and Oklahoma will perform research-level experiments in Heyes' lab.

News from Fulbright IT

Ronesha Sharma, Fulbright IT employee and undergraduate ISYS student from Walton College of Business, will be awarded $750 through the Destination z Enterprise Scholarship from IBM. Out of 10 recipients she is ranked number 4 on the list and was awarded one of the top three dollar amounts. "Watching Ronesha's skills and motivation grow have been an exciting journey. She shows enthusiasm with both her education and her work. We are very fortunate to have her on our team while experiencing academic success simultaneously," said Teresa Waddell, Director of Technology in Fulbright.

Ronesha Sharma

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LESLIE JOHNSON, EDITOR

Mailing Address
CHEM 119
1 University of Arkansas
Fayetteville, AR 72701

Phone: 479-575-4601
Fax: 479-575-4049
E-mail: cheminfo@uark.edu

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&
Department of Chemistry and Biochemistry *University of Arkansas

Safety Tip:
by Bill Durham

Disposable pipette tips should be collected in a labeled container that can be sealed with a lid when full (e.g., plastic gallon jugs). When the container is full, it should be placed directly in the dumpster. Individual tips should not be placed in the trash receptacles in the laboratories.

Department of Chemistry and Biochemistry

Excellence in the Central Science

Milestones

Graduate students Brett Spahn and Liz Srader were married January 5, 2013. The ceremony was held in historic downtown Rogers, Arkansas and they honeymooned in Montego Bay, Jamaica.

Brett is a Masters student and Liz is a Ph.D. student. Both are in the Gawley lab.

ARKANSAS INBRE
IDeA Networks of Biomedical Research Excellence

Save the Date!
The 2013 INBRE conference will be held October 18-19 in Fayetteville, AR.

2012-2013 CUME Schedule

All cumes are in CHEM 144, 5-6 p.m.

September 14	January 25
September 28	February 15
October 19	March 8
November 9	March 29

The department of chemistry and biochemistry at the University of Arkansas strives for excellence in research, teaching and service in chemistry - the central science. We aspire to positions of leadership regarding the discovery of new scientific knowledge, the training of students, and the economic development of the State of Arkansas. We seek to recruit and retain a diverse group of the best faculty, students and staff to address the challenges of the future through interdisciplinary and multidisciplinary research and education.

Calendar of Events

February

04 Biophysical Society Meeting
15 CUME
18 Seminar, Dr. Hedi Mattousi, Florida State University
25 Seminar, Dr. Carey K. Johnson, University of Kansas

March

01 Graduate student proposals due to committees
04 Seminar, Dr. Alexei Demchenko, Univ. of MO—St. Louis
08 CUME
11 Seminar, Dr. Adrian Michael, Univ. of Pittsburgh
12 Seminar, Dr. Steven Burke, Univ. of Wisconsin (please note Tuesday date)
18 SPRING BREAK
25 Seminar, Dr. Guozhong Cao, Univ. of Washington

Library Hours

CHBC Library (CHEM 225)
http://libinfo.uark.edu/chemistry
575-2557

Spring Semester Hours, Jan. 14, 2013—May 12, 2013

Monday—Thursday	8 a.m.-5 p.m.
Friday	8 a.m.-6 p.m.
Saturday—Sunday	Closed

Exceptions to Regular Hours

Monday, Jan. 21 (MLK Holiday)	Closed
Friday, March 15	8 a.m.-5 p.m.
Monday-Thurs., Mar. 18-21 (Sp. Bk.)	8 a.m.-5 p.m.
Friday, March 22	Closed
Friday, May 10	8 a.m.-5 p.m.

The chemistry and biochemistry library resources can be accessed in the following LibGuides: http://uark.libguides.com/content.php?pid=110953. Please bookmark for future use.
Theses and dissertation resources can be found on the following LibGuide: http://uark.libguides.com/content.php?pid=123035 &sid=1057466.