

The Mole Street Journal

Department of Chemistry and Biochemistry

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June 2012

Special points of interest:

- Pulay receives NSF grant
- Dr. Jingyi Chen receives honor
- Graduate students defend
- INBRE students arrive

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Pulay Receives NSF Award

Peter Pulay has received a 3-year, \$321,000 award from the National Science Foundation, starting on June 1, 2012. The award is for the computational modeling of solutions. Theoreticians are now able to model small single molecules in the gas phase with high accuracy.

However, most chemistry takes place in solutions. Solvents, particularly polar solvents such as water, influence the chemistry of reactions profoundly. The computational modeling of solutions is difficult because a solution has no fixed geometry. To get a result corresponding to experiment, one has to average over an astronomical number of solvent configurations. The methods developed by Dr. Pulay and his coworker Dr. Janowski speed up this process greatly (by 4-5 orders of magnitude, perhaps more for larger systems). Dr. Janowski is the author of a new computer program for these calculations. The program runs in parallel on the University of Arkansas RAZOR supercomputer, acquired partly by NSF support and partly by support from the State of Arkansas. Dr. Janowski has previously created a parallel computer program for high accuracy quantum chemistry simulations (the Coupled Cluster method). One of his applications of this program to the controversial question of the benzene van der Waals dimer became the most highly cited paper in *Chemical Physics Letters* in the 5-year period between 2006 and 2010.

Dr. Pulay is now in Kobe, Japan, the home of the currently largest supercomputer in the world, the K-computer which broke the barrier of 10 petaflops per second (1 peta=10 to the 16th power). He is a guest of Professor K. Hirao, a leading Japanese theoretical chemist and the director of the RIKEN Advanced Institute for Computational Science. He will return to Arkansas in early June.



Departmental Canoe Trip

The department took its yearly canoe trip on May 15, 2012. They paddled from Pruitt to Hasty on the Buffalo River.



Faculty News

On the Go

Charles Wilkins attended the 60th Conference on Mass Spectrometry Workshop May 24, 2012 and presented "The Use of Shape Selective Tandem Mass Spectrometry in the Characterization of Complex Formulations Containing Polymeric Components," coauthored by James Scrivens, Charlotte Scarff and Jonathan Snelling.

Matthias Knust presented a poster "FTMS Studies of the Influence of Plasma Gas Composition on Acetylene Gas Phase Polymerization," coauthored by **Charles Wilkins**, Carmen Santos, and Stephane Lucas.

Ingrid Fritsch presented an invited talk "Switching Active Electrodes to Maximize and Sustain Redox-Magnetohydrodynamic Microfluidics," coauthored by **Melissa C. Weston**, **Christena K. Nash**, and **Jerry Homesley**, at the 212th Meeting of the Electrochemical Society in Seattle, WA, May 6-10, 2012. Also presenting at that meeting was **Christena Nash**, who gave a talk, "Redox Polymer-modified Electrodes for Magnetohydrodynamic Pumping Systems." It was coauthored by **Ingrid Fritsch**. **Vishal Sahore** presented "Investigation of Redox Magnetohydrodynamic Microfluidics towards Lab on a Chip Assay Applications," coauthored by **Ingrid Fritsch**, at the Biosensors

2012 Meeting in Cancun, Mexico, May 15-18, 2012.

Publications

New Structural Insights into Mechanically Interlocked Polymers Revealed by Ion Mobility Mass Spectrometry. Charlotte A. Scarff, Jonathan R. Snelling, **Matthias M. Knust**, **Charles L. Wilkins**, and James H. Scrivens. *J. Am. Chem. Soc.* <http://pubs.acs.org/doi/abs/10.1021/ja2118656>.

Gramicidin A Backbone and Side Chain Dynamics Evaluated by Molecular Dynamics Simulations and Nuclear Magnetic Resonance Experiments. II: Nuclear Magnetic Resonance Experiments. **Vitaly V. Vostrikov**, **Hong Gu**, Helgi I. Ingolfsson, **James F. Hinton**, Olaf S. Andersen, Benoit Roux and **Roger E. Koeppe II**. (2011) *J. Phys. Chem. B*, 115, 7427-7432.

The Membrane Interface Dictates Different Anchor Roles for "Inner Pair" and "Outer Pair" Tryptophan Indole Rings in Gramicidin A Channels. **Hong Gu**, Kevin Lum, Jung H. Kim, **Denise V. Greathouse**, Olaf S. Andersen and **Roger E. Koeppe II**. (2011) *Biochemistry* 50, 4855-4866.

Response of GWALP Transmembrane Peptides to Changes in the Tryptophan Anchor Positions. **Vitaly V. Vostrikov**, **Roger E. Koeppe II**. (2011) *Biochemistry* 50, 7522-7535.

Thiazolidinedione Insulin Sensitizers Alter Lipid Bilayer Properties and Voltage-Dependent Sodium

Channel Functions. Rada Rusinova, Karl F. Herold, Lea S. Sanford, **Denise V. Greathouse**, Hugh C. Hemmings, Jr., and Olaf S. Andersen. (2011) *J. Gen. Physiol.* 138:249-270.

Membrane Binding of an Acyl-lactoferricin B Antimicrobial Peptide from Solid-state NMR Experiments and Molecular Dynamics Simulations. T.D. Romo, Laura A. Bradney, **Denise V. Greathouse**, and Alan Grossfield. (2011) *Biochim. Biophys. Acta.* 1808:2019-2030.

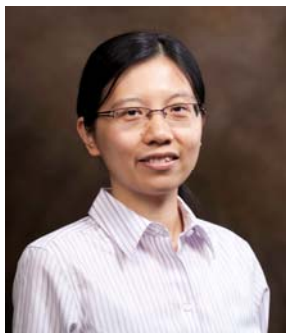
Linear Rate-equilibrium Relations Arising from Ion Channel-bilayer Energetic Coupling. P. Griesen, K. Lum, M. Ashrafuzzaman, **D.V. Greathouse**, O.S. Andersen and J.A. Lundabaek. (2011) *Proc. Natl. Acad. Sci., USA.* 108:12717-22.

On the Combined Analysis of ^2H and $^{15}\text{N}/^1\text{H}$ Solid-State NMR Data for Determination of Transmembrane Peptide Orientation and Dynamics. (2011) *Biophys. J.* 101, 2939-2947.

Tyrosine Replacing Tryptophan as an Anchor in GWALP Peptides. **Nicholas J. Gleason**, **Vitaly V. Vostrikov**, **Denise V. Greathouse**, **Christopher V. Grant**, Stanly . Opella, **Roger E. Koeppe, II**. (2012) *Biochemistry* 51, 2044-2053.

Proline Kink Angle Distributions for GWALP23 in Lipid Bilayers of Different Thicknesses. **J. M. Rankenberg**, **V.V. Vostrikov**, C.D. DuVall, **D.V. Greathouse**, **R.E. Koeppe, II**, **C.V. Grant** and S.J. Opella. (2012) *Biochemistry* 51, in press. <http://dx.doi.org/10.1021/bi300281k>.

Chen Selected to Connor Faculty Fellows



Jingyi Chen was selected to the 2012 class of Connor Faculty Fellows. Ten outstanding assistant professors were awarded this honor and given funds to support their career advancement in recognition of the outstanding teaching, research and service they provide to the college. Robert and Sandra Connor of Little Rock established the Connor Endowed Faculty Fellowship

in 2004 to provide essential faculty development opportunities to rising academic experts in the college. This award is used to facilitate travel, expand research initiatives and support classroom experiences.

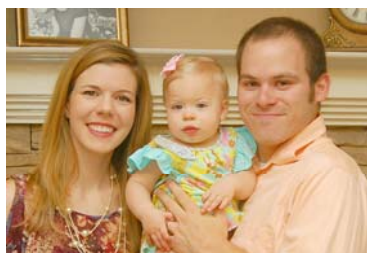
Students Defending

Zheng Li of Shanghai, China, defended his Ph.D. dissertation "Semiconductor Nanocrystals: From Quantum Dots to Quantum Disks" May 1, 2012. His advisor is Xiaogang Peng. Li has a B.S. in Chemistry from Hunan University and a M.S. degree from Fudan University, both in China.



Nicole Vanderbush of Senoia, Georgia defended her Ph.D. dissertation "An Analysis of the Redox Properties and Stability of *Chlamydomonas Reinhardtii* Cytochrome F, Cytochrome C₆, and Mutants Thereof" May 4, 2012. Her advisor is Dan Davis. Vanderbush has a biology degree from Shorter College. She is the daughter of Ricky and Linda Vanderbush of Senoia.

Nick Gleason of Austin, Arkansas defended his Ph.D. dissertation "Investigations of Protein-Lipid Interactions in Model Membranes: Influence of Aromatic Anchoring Residues and Buried Polar Residues" May 14, 2012. His advisor is Frank Millett. He held a Doctoral Academy Fellowship and the Barrett S. and Peggy S. Duff Doctoral Fellowship while pursuing his degree. Gleason has a B.S. in Chemistry from the University of Central Arkansas. He is married to Jamie Gleason and has a daughter, Lorelei.



Front (L-R): Indira Prajapati and Nicole Turnage
Back (L-R): Kai Carey, David Paul and Harold Owiti

The department welcomes to campus our summer **INBRE** student researchers. Kai Carey, from the Bahamas, is a student at Philander Smith College and is working with Dr. Yuchun Du in Biological Sciences. Harold Owiti is from Kenya and is a student at Williams Baptist College. He is working with Dr. Fiona Goggin in Entomology. Nicole Turnage is from Greenbriar Arkansas and is a student at Arkansas Tech. She is working in Chemical Engineering with Dr. Christa Hestekin. Indira Prajapati, from Nepal, is a student at Bethune Cookman and is associated with the George Washington Carver Research Program. She is working with Dr. David Paul in Chemistry.

Milestones



Pictured above are Asher and Clara Marissa Johnson, grandchildren of Lorraine Brewer and children of her daughter Amanda and son-in-law Brian. Clara was born March 9, 2012, weighed 7 lbs, 14 oz., and was 21" long.

Brett Spahn and Elizabeth Sradler, below, became engaged on May 17 at South Padre Island. They are planning an early January 2013 wedding.



Heather Jorgensen, Administrative Support Supervisor for the Dept. of Chemistry and Biochemistry, participated in the May graduation ceremony. She will complete her M.Ed. Degree in Higher Education Administration in July.

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Safety Tip: by Bill Durham

Small scale is the best approach when approaching a new reaction, especially one involving hazardous reagents.


Department of Chemistry
and Biochemistry

Excellence in the Central Science

Admitted to Candidacy



Brian Walker passed the required number of cumulative exams and was admitted to candidacy May 16, 2012. Brian is from Tulsa, OK and received his B.S. from James Madison University in Harrisonburg, VA and his M.S. from the University of Tulsa, OK. He is a member of the McIntosh lab.



Save the Date!

The department is again co-hosting the INBRE conference October 5-6, 2012 with the departments of biological sciences and physics. Events include faculty talks, student oral presentations, workshops, and a poster session. More information to come soon!

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

June

- 04 Classes begin for SS IV & V
- 06 Last day to drop SS V class without a "W"
- 12 Last day to drop SS IV course without a "W"
- 18 Last day to drop a SSI class with a "W"

July

- 01 Application deadline with the Registrar for August 2012 diploma
- 04 Independence Day, University closed
- 25 David Clay defends
- 27 Dissertation due in Grad School for August 2012 diploma

Library Hours

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

May 12-20 Monday-Friday 8 a.m.-5 p.m.

May 21 Summer Hours

Monday-Thursday 8 a.m.-6 p.m.
Friday 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>.

