

THE NEWSLETTER OF THE DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY



From the Editor:

In order to catch up on all of our happenings, The Test Tube will be divided into two volumes. Volume A will contain material from 2006-2007. Volume B will contain material from 2008-2009.

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* ACS SWRM - 2007 *

The American Chemical Society's 63rd Southwest Regional Meeting was held in Lubbock from November 4-7, 2007. There were 16 scheduled symposia, including a Tribute to Dr. G. Wilse Robinson, organized by Mostafa El-Sayed and Graham Fleming. All sessions took place at the Holiday Inn Park Plaza, and included socials, a winery tour and tasting, an awards banquet, and K-12 education events. The turnout was excellent, in large part to the SWRM committee members, and many in the

Transition States

department participated. Because of the high volume of



involvement by faculty and graduate students, we recommend you visit the official SWRM 2007 website to see all of the abstracts and presentations:

www.depts.ttu.edu/chemistry/SWRM07

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The Chair Conformation

Hi Everyone!

First, an apology...We started putting this edition of the Test Tube together immediately after the last one came out. Things have been so busy around here and there has been so much activity (in a great way!) that we (read I) weren't able to complete it in a timely fashion. Then, as more and more needed to be added, we realized a few months ago that it would be electron overload to try to put everything together into a single issue. So... we are putting this issue out before the end of the year to cover until the end of 2007. By March of 2010 we will put out a second issue that will cover until the end of 2009. We are then considering (since this now largely



Dr. **Robert Holwerda** poses with a stuffed penguin, one of the gifts presented to him during the Departmental Awards Luncheon for his 33 years of service to the department.

goes out electronically) sending out "Test Tubelets" once every three months (four times a year), instead of the usual annual newsletter. Things are changing that quickly around here...

Over the course of the time covered in this issue there have been a number of changes in the department. On the faculty front, Dr. Robert Holwerda retired in May of 2007 (Bob is still around as an emeritus faculty member) and Henry Shine "retired" for the third time (one of the things that Henry plans to do is to update the memoir that he previously wrote concerning the department, and which many of you have commented upon. It is located on our website if you haven't seen it). I, for one, hope that Dr. Shine continues to "retire" as many times as he would like!... Dr. Shaorong Liu headed off to the University of Oklahoma in early 2007. "Sooner" or later it had to happen (the good thing about electrons rather than paper is that they can't be used to smack me for my bad puns...). Cheryl Blasingame, our Administrative Assistant, moved on to another position on campus, as did Kathy Jones, our Graduate Advising Assistant. Many of you will remember how helpful both Cheryl and Kathy were in your careers. Adelina Loya, our Receptionist and the front face for the department, retired in early 2008. We wish her well as she spends more time with her family.

Many new faces also joined us through 2007. We hired a new Administrative Assistant, **Tammy Branham**, from the College of Business Administration, as well as a new Graduate Advisor, **Mary Beth Abernathy**, whom some of you will remember as the former Administrative Assistant in Chemical Engineering. We also hired a new Receptionist, **Melissa Graehling**, who came to us after several years in the cotton industry, and a new machinist, **Scott Hiemstra**. Scott is a true scholar-machinist. Besides being able to fabricate almost anything this side of 100 nm, Scott also frequents our departmental seminars (his undergraduate degree is in Physics, but we don't hold it against him!...)

We'll update you on all of the other news that has happened since 2007 in our next issue. A teaser, though... Almost all of these folks are

now (2009) in different positions in our department and across the university! I told you things are moving fast around here, almost as fast as a picosecond electron transfer process!

One of the more exciting aspects of the 2007 year was the development and first meeting of the Department of Chemistry and Biochemistry's Chair's Council. The Chair's Council is an advisory group for the department composed of 12-15 individuals who are graduates or long-time supporters of the department who have gone on to neat careers and who have agreed to a three-year commitment to provide advice to the department on how to move to the next level in all phases of department activity. They have already done

some amazing things for the department with regard to helping us overhaul our graduate program and fundraising. I hope that all of you TTU Chemistry and Biochemistry fans (you wouldn't be getting this newsletter if you weren't!) will consider a stint on the Council.

For now, happy holidays, and may your reactions be merry and bright!

Dominich J. Cossolante. Jr.

Dom Casadonte Professor and Chair



(L to R): The "Freebases", the Chemistry Softball Team after one of their first games in June 2007. Pictured here: Kulothungan Ganapathy, Patrick McLaurin, David Snow, Charlotte Sisk, Michael Jones, Dominick Casadonte, Dylan Drake-Wilhelm, Tina Thomas, Amanda Boston, and Brandon Berkshire.

Staff Role Call

We have had several staff changes over the past few years. Cheryl Blasingame moved across campus to work for PrintTech, and Kathy Jones moved to the Health Sciences Center. Rachel Clark, Cheryl Essery, Adelina Loya, Brandon Sheehan, Judy Payne, Duane Hindes, Mary Beth Abernathy, Tammy Branham, and Pam Cox have also left the department. Our newest staff members are **Josie Aguilar**, Receptionist; **Carly Jenkins**, Senior Business Assistant -Academic Office; **Peter O'Connell**, Machinist; and **Mayela Sanchez**, Senior Business Assistant -Administrative Office.

In other news, **Nina Pruitt** was a recipient of the 2007 Texas Tech Alumni Association's Top Techsan Award. She was presented with a plaque, monetary award, and was introduced on the football field during halftime at the 2007 Homecoming game in October. Congratulations, Nina!



(L to R): Dr. **Louisa Hope-Weeks** stopped by the Business Office with her newborn, Rhiannon. **Kathy Jones** receiving her going away gift at the Departmental Holiday Lunch. **Nina Pruitt** stands with her husband J.D., daughter in-law Whitney Meadows, and son Kirk Meadows at the Texas Tech Alumni Association's Top Techsan Award Ceremony where Nina was presented with a plaque and monetary award.

Family Matters

Debbie Martinez and her husband Bryant, are proud to announce the birth of their son, Raydan Joe. He was born at 6:34 pm on December 13, 2007. He weighed 7 lbs, 8 oz and was 20 inches long.

Dr. **Louisa Hope-Weeks** and her husband, Brandon Weeks, have a new baby girl. Rhiannon Mary Weeks was born at 2:28 am on Sunday, September 2, 2007. She weighed 8 lbs, 13 oz and was 21.5 inches long.

Patrick McLaurin and his wife, Latisha, are proud to announce the birth of their daughter, Calista Anne. She was born June 1, 2007 at 1:57 pm. She weighed 6 lbs, 4 oz and was 19.5 inches long.

Jeremy Mason and his wife, Sara, have a new baby girl as well. Mackenzie Chiyomi was born January 12, 2007 at 6:13 pm. She weighed 5 lbs, 13 oz and was 20 inches long.

Congratulations to all of the proud parents and their new family additions!

Current Departmental Staff

ACADEMIC OFFICE Melissa Graehling Carly Jenkins LaQuetta Purkiss

ADMINISTRATIVE OFFICE

Nina Pruitt Josie Aguilar Mayela Sanchez

BUILDING AND SHOPS Scott Hiemstra Jim Hildebrand Peter O'Connell Jerry Walton Vince Wilde

<u>BUSINESS</u> OFFICE Yesenia Sanchez Rosa Maria Diaz Glenda Schaefer GLASS SHOP Don Hodgkins

INFORMATION OFFICE Whitney Green

MASS SPECTROMETERS Kazimierz Surowiec

<u>NMR SPECTROMETERS</u> David Purkiss

> STOCKROOM Justo Adame Debbie Martinez

<u>WELCH OFFICE</u> Sophie McDougal

In Memoriam

Mr. **Noah Hernandez Solis**, our part-time machine shop technician, passed away Tuesday, March 27, 2007. After many years with Building Maintenance, Noah retired from TTU in 1992. He worked part-time for the department from July 1992 through March 1993 to help out while a technician was on a leave of absence. The department hired Noah again in 1997. Noah was born Sept. 4, 1931, in Kosse, TX to the late Ventura and Petra Solis. He served in the US Army during the Korean War. Noah pastored and ministered with the Assemblies of God. He also worked at Texas Tech University as a machinist, a job he held for more than 35 years.

Dr. **Dennis C. Shelly** passed away on Friday, November 21, 2008, in College Station, as a result of a motor vehicle accident. Born on Feb. 16, 1955, in Chambersburg, PA he was the son of Harry C. and Joan L. Armstrong Shelly.

A 1973 graduate of James Buchanan High School, he attended Huntington College, Huntington, Ind. and received a Bachelor of Science Degree in Chemistry. In 1982, he received a Doctor of Philosophy degree in Analytical Chemistry from Texas A&M University, College Station. Following graduation he worked for Eli Lilly and Co., Indianapolis, Ind. Realizing that he wanted to teach he accepted a post-doctoral fellowship at Indiana University, Bloomington, Ind. Following his post-doctoral fellowship he taught chemistry as an assistant professor at Steven's Institute of Technology, Hoboken, N.J. In 1990, he accepted a position at Texas Tech University teaching chemistry.

Dennis had a passion for leather research and was president of the Leather Research Institute at Texas Tech University. He was also a past president and active member of the American Leather Chemists Association. His long-standing organizational memberships included the Leather Industries of America, Society of Applied Spectroscopy and American Chemical Society.

Dennis was a well-respected leather researcher throughout the world. In addition to his research abroad, he often lectured and presented seminars in China, India, Vietnam, Eastern Russia and the United States. In 2005, Dennis was the recipient of the distinguished Alsop award for outstanding scientific contributions to the leather industry.

Dr. **John L. Kice**, former Chemistry Chair at TTU, died in Aurora, CO, on October 31, 2008.

Kice joined TTU's department as chairman in 1975. He served briefly also as associate dean for research. In 1985 Kice left TTU to become chairman of chemistry at Denver University, returning thereby to the State in which he was born and for whose mountains he had never lost his love. At DU he moved in 1988 from chemistry chair to dean of Natural Sciences, Mathematics and Engineering. He retired from DU in 1995.

Kice received the AB (1950), MA (1953), and PhD (1954) degrees from Harvard, which he entered at the age of 15. During 1957-1961 he was an Alfred P. Sloan fellow. Before joining TTU he held positions at the University of Vermont, Oregon State University, and the University of South Carolina.

Kice was an eminent physical organic chemist, specializing in organosulfur chemistry, particularly in the reactions of disulfides, sulfinic acids, sulfinyl sulfones and related compounds. He was a gifted teacher and writer of textbooks, among them being "Modern Principles of Organic Chemistry (with E. N. Marvell) in 1966, and "Organic Chemistry" in 1982.

We will remember him at TTU as our first chairman brought from outside the department, devoted to serving the department and a splendid colleague.





(T to B): Dr. **Dennis Shelly** standing on a shoreline, September 2007. **"Mac" McPherson**, **Henry Shine** and **John Kice** at a reception in December 1983.

Photos from the 2007 ACS Southwest Regional Meeting



Chair's Council Founding Members



Dr. Avens



Dr. Heineman



Dr. Babb



Dr. Henry



Dr. George



Dr. Kemp



Dr. Gilbert







Dr. Goodin



Dr. Robinson



Dr. Harwell



Dr. Seale

Robinson Lecture

The Fifth G. Wilse Robinson Endowed Lecture Series were held on Thursday, March 22, 2007 and Friday, March 23, 2007. During these two days, Dr. Peter G. Wolynes gave two seminars. His public lecture was entitled "Landscapes of the Sciences," and his technical talk was "Energy Landscapes and Solved Protein Folding Problems."

Dr. Wolynes is the Francis Crick Chair in Physical Sciences in the Department of Chemistry and Biochemistry at the University of California, San Diego. He received his A.B. degree in 1971 from Indiana University. He then took up the study of statistical mechanics at Harvard, where he received his Ph.D. in Chemical Physics in 1976. In addition to continuing his work on many body chemical physics and protein folding, he is now studying stochastic aspects of cell biology.

Shine Lectures

The Seventh Henry J. Shine Lecture Series were held Tuesday, October 23, 2007 and Wednesday, October 24, 2007. Professor Jacqueline K. Barton was the special guest speaker and gave two seminars. Her public lecture was entitled "Travels Along the DNA Helix: A Different Perspective," and her technical talk was "DNA Charge Transport Chemistry & Biology."

Dr. Barton is the Arthur and Marian Hanisch Memorial Professor of Chemistry at the California Institute of Technology. Barton was awarded the A.B. summa cum laude at Barnard College in 1974 and a Ph.D. in Inorganic Chemistry at Columbia University in 1978 in the laboratory of S. J. Lippard. She has received numerous awards; among the most recent are the ACS Breslow Award in Biomimetic Chemistry (2003), the ACS Gibbs Medal (2006), the ACS Cotton Medal (2007), and the ACS Pauling Medal (2007). She is also a member of the National Academy of Sciences (2002).



(Above:) Dr. Henry Shine stands with his wife, Sellie, Dr. Barton and Dr. David Birney.
(Below:) A huge turnout for the 8th Shine Lecture Series. Drs. Mayer, Fuertes, Birney, Hope-Weeks,
Casadonte & Niwayama stand with Dr. Grubbs.

The Eighth Henry J. Shine Lecture Series were held Tuesday, March 4, 2008 and Wednesday, March 5, 2008. Professor Robert H. Grubbs was the special guest speaker. His public lecture was entitled "From fundamental research to applications: The olefin metathesis reaction." His technical talk was "The design and synthesis of new olefin metathesis catalysts."

Dr. Grubbs received his B.S. in Chemistry from the University of Florida in 1963 and his M.S. with Merle Battiste in 1965. His Ph.D. was with Ronald Breslow at Columbia University, in 1968. He is currently the Victor and Elizabeth Atkins Professor of Chemistry at the California Institute of Technology. His many awards have included ACS National Award in Organometallic Chemistry (1988), ACS Arthur C. Cope Award (2002), Pauling Award Medal (2003), and the Nobel Prize in Chemistry (2005). He was elected to the National Academy of Sciences in 1989.





Transition States: Graduations

PhD Degree in Chemistry

December 2006

Rukma Basnayake (Analytical-Korzeniewski)

Strategies for Probing Platinum-Based Electtrocatalyst and Ionically Conductive Membrane Materials: Voltammetry of Platinum Ruthenium and Platinum Vandium Nanoparticles and Infrared Studies of Membrane Hydration

Lin Gao (Analytical-Liu)

Development of Cross-Linked Polyacrylamide Coating for Protein Separations by Capillary Electrophoresis

Pruthvi Jayasimha (Biochemistry-Nes)

Sterol Methyltransferase: Protein Engineering, Molecular Mapping of AdoMet-Binding Site, Thermodynamic Analysis and its Phylogenetic Implications Dongmei Zhang (Organic-Bartsch) Synthesis of New Proton-ionizable Multidentate Ligands

May 2007

Ademola David Idowu (Analytical-Dasgupta) Measurement of Arsenic in Water and Soil Based on Gas-Phase Chemiluminescence

Jing Wang

(Analytical-Bartsch) Metal Cation Complexation by Multidentate Ligands

Yining Wang (Organic-Li) Regio- and Stereoselective Functionalization of Olefins



August 2007

Yining Liu (Analytical-Dasgupta) Determination of Iodide and Iodate in Aqueous Solution

Matthew Phillip Soape (Biochemistry-Nes)

Protein Chemistry, Peptide Mapping, and Preliminary Structural Characterization of Saccharomyces cerevisiae Sterol C-24 Methyltransferase Expressed in Escherichia coli

August 2007

Yingsheng Xiao (Physical-Poirier)

Efficient Full Quantum Calculations for Small Molecules Using Novel Phase Space Optimized Discrete Variable Representation Path Integral Monte Carlo Methods

Huiming Zhang (Biochemistry-Paré)

Mechanisms for Plant Growth Promotion Trigged by Bacterial Volatiles

December 2007

Venkata Adiseshu Kattubboina (Organic-Li)

Development of Chiral N-Phoshpony Imines Chemistry and New Tandem Bond-Formation Reactions

Shengfu Li (Organic-Bartsch)

Synthesis, Properties, and Applications of Ionic Liquids

December 2007

Bipasha Deb (Physical-Hase)

Potential Energy Function and Dynamics of Energy Transfer and Fragmentation for Collision of Profonated Peptide Ions with Organic Surfaces

Indra Sena Reddy Gudipati (Organic-Birney)

Microwave Assisted Generation and Tripping of Acetylketene

Prasanth Pathange (Biochemistry-Shi)

Characterization of an Abiotic-Stress Responsive Sulfotransferase Gene from Arabidopsis

Masters Degree in Chemistry

December 2006

Gaurav Harish Kumar Arora (Organic-Bartsch) Calix[4]arenes with Proton-ionizable Groups on the Lower and Upper Rim

May 2007

Xiaodan Cao (Analytical-Bartsch) Evaluation of Multidentate Ligands in Ion-Selective Electrodes

Bachelor of Arts in Biochemistry

December 2006

Debra Nnedinma Osadebe Erin Michelle Wolf

May 2007

Mike Preston Berry Brittany Leilani Davis Adrienne Sarah Hiatt Michelle Leigh Ivey Joseph Trent Marino Shaughn Michale Nunez Colbert Rick Perez Derek Lee Piaschyk

Bachelor of Arts in Chemistry

December 2006

Emilia Kate Arguello Dana Michelle Heathington Tiffany Lauren Patterson Michael William Rice

Bachelor of Science in Biochemistry

December 2006

Carlos Angel Bergfeld Emily Jo Hall Katelyn Rhea Halley Katelyn Rhea Halley Benjamin David Nelson

May 2007

Jacob Lee Hopkins Kristopher Kyle Koelker Kyle Ray Miller Lindsay Kate Nichols Mark Brandon Nix Michael Kariuki Njenga Hal Gregory Penchan Arvin Khorrami Zeinali

May 2007

Phuong Tram Dang Jack William Drakeford Stefan John Friemel Anushre Gupta Anthony James Lewis Juia Claire McLouth Shawna Gail Thomas Trevor Grant Wall Jennifer Sarah White Matthew Wayne Wilson Susan Ellen Wozniak Dora Irina Zanescu

August 2007

Ehihimen Osioriamen Okogbo Brooks Michael Stevens

December 2007

Sarah Marie McRae Mary Ann Mullen Jessica Renee Solis

August 2007

December 2007

Samuel Duane Edwards Heather Marie Naegeli Joshua Christian Nittinger Ashley Dyan Webster

August 2007

Leslie Michelle Perry Beau David Stephenson

December 2007 -----

Bachelor of Science in Chemistry

December 2006

May 2007

Dawn Ellen Cline Janette Cortez Uwana Ndanyongmong Ibanga Geneva Ruth Peterson Matthew Alexander Reyes

August 2007

Evan Ross Adams Nicholas Ryan Delone Christianah Aderonke Layode Puhui Li Cynthia Sue Nesmith Andrew Michael Shobe

December 2007

Travis Daniel Alexander Griselda Garza Tyler Reid Harrington Careen Elizabeth LeMeilleur Molly Kate Marshall

Congratulations, Graduates!

Faculty News & Notes

Richard A. Bartsch, Analytical and Organic:

- * received a three year renewal grant for the amount of \$150,000 from The Welch Foundation for "Synthetic Hosts for Recognition of Ionic and Molecular Guests".
- * presented two papers in the Symposium on Calixarenes: State of the Art and Perspectives on March 26, 2007 at the 233rd National Meeting of the American Chemical Society in Chicago. The ACS Division of Industrial & Engineering Chemistry organizes this symposium.

Robert E. Blake, Jr., Chemical Education:

- * coordinated the Chemistry Scholars Program. The Chemistry Scholars, chosen from the pool of undergraduate Chemistry and Biochemistry majors, led discussion sections for CHEM 1301, Introductory Chemistry. The student leaders are eager about the opportunity to solidify their fundamental chemistry understanding and help their peers, and Dr. Blake is thrilled to see students excited about learning chemistry!
- * organized a symposium "Research in Chemical Education" at the American Chemical Society Fall National meeting in Boston, served on the State of Texas content validation committee for the TAKS examination in chemistry, authored a chapter in a textbook, and played bass guitar in a local band.

Dominick J. Casadonte, Jr., Inorganic:

- * was honored at Mortar Board's annual Apple Polishing ceremony. The reception is a way for Mortar Board Members to say thank you to faculty for their work and dedication as teachers. Mortar Board is a national senior honor society representing the best and the brightest seniors across the United States.
- * was recognized by the 2007 Texas Tech University chapter of Phi Beta Kappa as an outstanding professor.

Michael J. Fuertes, Organic:

- * was awarded a new three year grant of \$150,000 by the Welch Foundation for his proposal entitled "New Metal-Mediated Strategies for the Stereoselective Synthesis of Highly Functionalized Cyclic Ethers and Piperidines."
- * was recognized by the 2007 Texas Tech University chapter of Phi Beta Kappa as an outstanding professor.







(T to B): Dr. **Richard Bartsch**, Shannon Keel, President Jon Whitmore, and Dr. **Henry Shine** at the Welch Banquet. Dr. **David Birney** and graduate student **Hua Ji** at SWRM ACS Meeting. Drs. **Michael Mayer, Michael Fuertes**, and **Dominick Casadonte** after the Shine Lecture.

William L. Hase, Physical:

- * was named Lead PI of a Partnership in International Research and Education (PIRE) grant awarded to Texas Tech University by the National Science Foundation. The award is \$500,000/year for five years. The title of their project is "Simulation of Electronic Non-Adiabatic Dynamics for Reactions with Organic Macromolecules, Liquids, and Surfaces" and their collaborators are at Iowa State University, Yale University, University of Santiago de Compostela (Spain), University of Pisa (Italy), and University of Vienna (Austria).
- # gave several invited lectures throughout 2007. They included: "Direct Dynamics Simulations of Gas Phase Ion-Molecule Reactions" at the 9th Gordon Conference on Structures, Energies, and Dynamics of Gaseous Ions held in Ventura, California, February 25 - March 2; "Simulations of Interfacial Structures and Dynamics" in the Symposium entitled Capturing Complexity in Physical Sciences Simulation at the 222nd National Meeting of the American Chemical Society held in Chicago, Illinois, March 25 - 29; "Energy Transfer in Collisions of Projectiles with Organic Surfaces" at the 20th International Conference on Molecular Energy Transfer held in Arcachon, France, June 3 - 7. He also gave the seminar "Dynamics of Energy Transfer and Fragmentation in Surface-Induced Dissociation of Protonated Peptide Ions" at the Universidad de Santiago de Compostela, Spain on May 31.
- * is one of eight co-organizers for the 2008-2009 thematic year for the Institute for Mathematics and its Applications (IMA), at the University of Minnesota, which is funded by the National Science Foundation. The theme for 2008-2009 is "Computational Chemistry". Several Workshops will be held during the year, and from January 12-16, 2009, Dr. Hase will be leading the organization of a workshop entitled "Chemical Dynamics: Challenges and Approaches".

David B. Knaff, Biochemistry:

- * was named Co-PI for a \$499,692 grant from the VP for Research and Development supporting intramural research between the main campus and the TTU Health Sciences Center. The three-year project is entitled "A New Proteomics Method and Its Application to Chemical Biology".
- * has been selected as the 2007 recipient of the ARCS (Achievement Rewards for College Scientists) Foundation Inc. Scientist of the Year Award. The ARCS Foundation is dedicated to helping meet the country's need for scientists and engineers by providing scholarships and recognition to academically outstanding United States citizens who complete their degrees in science, engineering, and medicine, thereby contributing to the worldwide advancement of science and technology. The Lubbock ARCS chapter is the only chapter in the state of Texas, and has awarded over \$1.4M to over 600 scholars since 1972.





(L to R): Dr. **Robert Holwerda** stands with his family at his retirement party. **Yesenia Sanchez** and **Nina Pruitt** pose with Drs. **David Knaff** and **William Hase** at the Henry J. Shine Lecture Series Reception.

Shaorong Liu, Analytical:

- * was named Co-PI for a \$499,692 grant from the VP for Research and Development supporting intramural research between the main campus and the TTU Health Sciences Center. The three-year project is entitled "A New Proteomics Method and Its Application to Chemical Biology".
- * was promoted to Full Professor and received tenure effective September 1st, 2007.

Jorge A. Morales, Physical:

- * was promoted to Associate Professor and received tenure effective September 1st, 2007.
- * obtained the grant "Combined Coherent-States/Density-Functional-Theory Dynamics" from the American Chemical Society Petroleum Research Fund (PRF), a PRF Grant Type A/C for \$80,000.00 for the period of July 01, 2006 to August 31, 2008.
- * presented the talk "Coherent-States Chemistry: A Unified Approach to Ab Initio Molecular Dynamics" on September 20, 2006.
- * was elected as a member of the Texas Tech University Teaching Academy in recognition of his teaching services and performance on October 12, 2006.
- * presented the keynote speech "Coherent-States Dynamics: A Tribute to N. Yngve Öhrn" at the Symposium in Honor of N. Yngve Öhrn, International Conference of Computational Methods in Sciences and Engineering 2007, Corfu Island, Greece, September 28, 2007. Parts of this talk have been published as a referred paper in the American Institute of Physics Conference Proceedings 963, 460-473, (2007).
- * presented the poster "Performance Comparison between our campus-wide desktop grid and Beowulf clusters in the simulation of the H+ + H2 at ELab = 30 eV reaction: A computational study with the electron nuclear dynamics theory" in collaboration with Mr. Jerry Perez at the TTU High Performance Computer Center and with other members in that division, at the International Conference for High Performance Computing Networking, Storage and Analysis, in Reno, NV on November 10, 2007.
- * received a prestigious National Science Foundation-Career Award. His NSF-CAREER proposal, "Building a Direct Dynamics with Coherent States" was approved for funding by NSF in a total amount of \$569,463.00 for five years, starting on February 1, 2007. Professor Morales is the second faculty member in the Department of Chemistry possessing the NSF-CAREER Award, and is the first one to have obtained such a distinction while being in the department since the beginning of his professional academic career. Professor Morales' NSF-supported research project is in the field of theoretical and computational chemistry and applies his novel coherent-states theories to chemical dynamics.





(L to R): Dr. **Carol Korzeniewski** and students from the 2007 "Science, It's A Girl Thing" program. Dr. **Jorge Morales** stands with Postdoc **Kakha Tsereteli** at the ACS's 63rd Southwest Regional Meeting.

W. David Nes, Biochemistry:

* was promoted to Paul Whitfield Horn Professor, effective September 1st, 2007.

Satomi Niwayama, Organic:

- * received the "ACS PROGRESS/Dreyfus Lectureship" Award, which is funded by the Camille and Henry Dreyfus Foundation Special Grant Program in the Chemical Sciences. This lectureship award is provided to a female tenured/tenure-track Assistant or Associate Professor who started her full-time appointment no later than September 2003 in a chemistry or chemical engineering department that offers a Ph.D. degree. This award provides a travel grant of up to \$1000 for the recipient to present her research at Carnegie Research Extensive universities in the US. With this lectureship, Dr. Niwayama delivered seminars about her research at the University of Pennsylvania, Princeton University, Columbia University, New York University, and the State University of New York at Stony Brook in December.
- * received a TTU-TTUHSC Initiative grant as the lead PI from the TTU campus for research entitled "A New Proteomic Method and Its Application to Chemical Biology." The grant, which comes from the TTU Office of the Vice President for Research and TTUHSC Office of the Executive Vice President for Academic Affairs, is for \$499,692 for collaborative research, and involves Robert Bright (lead PI from TTUHSC), and Co-PIs, David Knaff (TTU), Shaorong Liu (TTU), Lauren Gollahon (TTU), Nathan Collie (TTU), and Gail Cornwall (TTUHSC). With this grant, Dr. Niwayama purchased a new mass spectrometer, MALDI TOF/TOF 4800 Plus from Applied Biosystems.
- * delivered seminars at Johns Hopkins University School of Medicine in May, at Shenzhen Graduate School of Peking University in China in July, Takeda Pharmaceutical Co. Ltd., in Japan in August, and four universities in Japan (Tokushima University, University of Shizuoka, Ochanomizu Women's University, Gunma University).

Dimitri Pappas, Analytical:

- * had a paper chosen as the featured article in the October 2007 issue of *Analytica Chimica Acta*. The paper, entitled "Isolation and counting of multiple cell types using an affinity separation device," was co-authored by graduate student, Kelong Wang, and Honors College undergraduate, Brandon Cometti. The Pappas group also published a review article in the same issue of the journal.
- received a three year grant in the amount of \$50,000 from the Welch Foundation for "Single Molecule Investigations of Energy Transfer and Light Harvesting of Phycobiliproteins."
 With this new grant, Dr. Pappas' students will investigate energy transfer of fluorescent protein complexes on the single molecule level.







(T to B): Dr. John Marx stands with the Science Fair Winners at the ACS Banquet. Drs. Richard Babb and Satomi Niwayama during her Industrial Chemistry Course. Drs. Guigen Li, Michael Jones, Dongmei Zhang, Michael Fuertes, Satomi Niwayama, Henry Shine, Richard Bartsch, David Birney and Michael Mayer raise a toast to Dr. Shine.

L. William Poirier, Physical:

* received a National Science Foundation Small Grant for Exploratory Research (SGER) entitled "Bipolar Quantum Trajectory Simulations". SGER applications, submitted only with approval of an NSF program officer, explore "high risk and novel ventures into emerging and potentially transformative research ideas, likely to catalyze rapid and innovative advances." Poirier's SGER project, a two-year grant in the amount of \$173,418, will develop numerical methods to incorporate quantum mechanical effects into existing classical simulations codes (already used in a great many scientific and engineering fields), thus allowing reliably accurate quantum calculations to be performed for large systems for the first time.

Edward L. Quitevis, Physical:

- * received notification that his proposal entitled "Understanding the Role of Nanostructural Organization in the Intermolecular Dynamics of Room Temperature Ionic Liquids," was recommended for funding by the American Chemical Society - Petroleum Research Fund Advisory Board for \$100,000 for two years starting January 1, 2008. Dr. Quitevis will study how the liquid structures that form on the nanoscale determine the intermolecular dynamics of these materials.
- * was awarded a three year grant in the amount of \$454,050 from the National Science Foundation for "Probing Nanostructural Organization in Room Temperature Ionic Liquids Using Optical Kerr Effect Spectroscopy". This proposal, which was sent to the highly competitive Experimental Physical Chemistry Program, is aimed at obtaining a fundamental understanding of the intermolecular dynamics of ionic liquids. These materials are of great interest in that they are "green" alternatives to volatile organic compounds (VOCs) used in chemical and industrial applications.
- * had a paper entitled, "Nanostructural Organization and Anion Effects on the Temperature Dependence of the Optical Kerr Effect Spectra of Ionic Liquids," chosen as one of 6 articles featured on the cover of *The Journal* of *Physical Chemistry B*, Volume 111, No. 18. The paper describes studies of the relationship between the structure and intermolecular dynamics of room temperature ionic liquids (RTILs). RTILs are of great interest in that they are "green" alternatives to volatile organic compounds (VOCs) used in chemical and industrial applications. *The Journal of Physical Chemistry B* has an ISI® impact factor of 4.115, highest among general physical chemistry journals.
- * gave an invited talk entitled "Effect of Symmetry of the Cation on the Intermolecular Dynamics and Physical Properties of Imidazolium Ionic Liquids," at the 2nd International Congress on Ionic Liquids in Yokohama, Japan on August 5-10, 2007.
- * gave invited lectures on "Nanostructural Organization in Ionic Liquids Probed by Optical Kerr Effect Spectroscopy " at Brooklyn College on October 22, at Johns Hopkins University on October 24, and on "Dynamic Heterogeneity and Translational and Rotational Diffusion in Glass-forming Liquids near the Glass Transition" at Rutgers University on October 23.



(Top to Bottom): Dr. **Henry Shine** stands with a cake honoring him for his many years with the department. Drs. **Bill Poirier, Henry Shine**, and **Paul Pare** at the Annual Welch Foundation's Banquet.



Robert W. Shaw, Biochemistry:

* received a \$63,000 grant through Texas Tech University's new \$100,000 Commercialization Accelerator Fund, which will help researchers through the final stage of work needed to apply for patents. He has developed a compound that could increase the effectiveness of current antibiotics. His work is protected by three patent applications. Dr. Shaw has developed an inhibitor compound that can be administered in combination with antibiotics to prevent the enzymes from inactivating the antibiotic allowing the drugs to kill the bacteria. He will use his grant for animal testing that will accelerate the commercialization of the technology.

Dennis C. Shelly, Analytical:

- * led the American Leather Chemists Association (ALCA) as it hosted the 29th Congress of the International Union of Leather Technologists and Chemists Societies (IULTCS). Their meeting was June 20-24 in Washington, D.C. and was also the 103rd Annual Meeting for the 400member American group, over which Shelly presides as President.
- * was invited to give a research paper at "Leather and Fur in the 21st Century". Sponsored by the East Siberian State University of Technology, the conference was held September 10-14, 2007 close to Lake Baikal in the tourist city of Ulan Ude, in the Republic of Buryatia. The paper was entitled, "An Inexpensive Shrinkmeter for Studies of Hydrothermal Mechanical Behavior of Wet Blue, Crust and Finished Leathers".
- * was part of a forum and panel discussion at the 7th China (Shiling) Leather and Its Products Fair on October 30-November 1 in Shiling, Guangzhou, China. Dr. Shelly spoke on the topic "Synergistic Partnerships Offer Sustainability" as he summarized recent successes in collaborating with government agencies, private industry, and producer groups as part of his leadership of Tech's Leather Research Institute. A second element of his presentation focused on characteristics of the American marketplace. Dr. Shelly's presentation was organized for the Second Global Leather Products Industry Development High Peak Forum.



Dr. **Dennis Shelly** stands next to an Asian statue. He was part of a forum and panel discussion at the "7th China Leather and Its Products" Fair in 2007.

Huazhong Shi, Biochemistry:

* was awarded a three year grant in the amount of \$349,143 from the United States Department of Agriculture National Research Initiative (NRI) Competitive Grants Program. The awarded project is "Characterization and Molecular Identification of sos1 Suppressors in Arabidopsis".

Joachim Weber, Biochemistry:

* published an original research paper in the *Proceedings of the National Academy of Sciences of the U.S.A.* entitled "Identification of the bTP site in the x-ray structure of F1-ATPase as the high-affinity catalytic site". An invited review, entitled "ATP synthase – the structure of the stator stalk" appeared in *Trends in Biochemical Sciences. PNAS* has an ISI® impact factor of 9.6; *TiBS* has an impact factor of 13.3.

Dongmei Zhang, Organic:

* became a member of the departmental teaching community. Her principle teaching and development duties are in Organic Chemistry, with an occasional course in General Chemistry as needed.



John Collette (BS Bich 1997) attended graduate school at the University of North Carolina at Chapel Hill where he received his Ph.D. in Biochemistry in 2004. He has been working for the past 2.5 years at the University of Miami School of Medicine. John is currently a postdoc in a lab in the department of Molecular and Cellular Pharmacology. In the summer of 2006, he received a two year postdoctoral fellowship from the American Heart Association to continue his scientific research pursuits at UM.

George Edwards (BA Chem 1951) went from Texas Tech to med school, practiced medicine for 37 years, and then retired.

Lin Gao (PhD Liu 2006) has joined The University of Mary Hardin-Baylor as an Assistant Professor.

Christi Gwyn (BS Chem 1997, MS Bartsch 2003) is getting married in may 2007 to Jeff Criswell of Amarillo

Ju-Guang Han (Postdoc Morales) was appointed as a faculty member at the Chinese Academy of Science National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, An-Hui Province, People's Republic of China.

Jason Montgomery (MS Poirier 2002) successfully defended his Ph.D dissertation at the University of Chicago. He now has a job as a postdoc at Argonne National Labs, working for Dr. Stephen Gray.

Paramashivappa Rangappa (Postdoc Shine) but I have just heard from him that he has changed his job. He is now a Research Scientist in the Drug Discovery Center of AstraZeneca India in Bangalore, India.

Carrie Lee (Bates) Sims (BS Chem 1999, MS Bartsch 2002) is living and working in the New Orleans Metro Area with her husband, Aaron. She is employed by Lockheed Martin and works at the NASA owned Michoud Assembly Facility where they manufacture the External Tank for the Space Shuttle. When not working, she and her husband enjoy playing soccer, walking their dog, serving in their church and traveling.

Byungki Son (PhD Bartsch 1985) returned to Korea and has been working in industry. While living in Lubbock, a son, Pillhun, was born to Byungki and his wife. This younger son is now graduating from Seoul National University, the top-ranked public university in Korea, with a degree in chemistry and will begin his doctoral degree studies in this department in August and will join the Bartsch research group.

Bing-Jun Zhao (Postdoc Shine) is now working in research with the Perkin-Elmer Co. in Boston, MA.





(L to R): **John Collette** and his wife, Rebekah, standing in a tailgating lot next to the Orange Bowl on Thanksgiving Day in 2006. **Pillhun** and **Byungki Son** in front of the Chemistry Department at Seoul National University, Pillhun is a member of Dr. **Bartsch's** group, just like his father who received his doctorate under Bartsch's supervision in 1985.

Cody Timmons (PhD G. Li 2006) is in a tenure-track faculty position at Southwestern Oklahoma State University near his hometown. Cody started there in August of 2007. He has less than one-year of postdoctoral experience at University of Pittsburgh; finding a faculty position at a non-Ph.D. institution has been his goal.

David Womack (BS Chem 1983) has been teaching high school for over 23 years. He spent a year in graduate school at Texas Tech, but developed a love for teaching through his experiences as a T.A. David taught two years at Lubbock High School, nine years at Cedar Hill High School, and has spent the last twelve years at Duncanville High School. He has taught Physical Science, PreAP Chemistry, and AP Chemistry, and is currently teaching PreAP Chemistry and AP Chemistry. I also serve as the UIL Science sponsor and the Student Council Advisor; so, my schedule is very busy! I consider myself very fortunate to be able to apply so much of what I learned at Texas Tech to my profession. I enjoy keeping up with events in the Chemistry Department through "The Test Tube." I hope the faculty will encourage outstanding students to consider careers in education, because our education system needs more dedicated teachers.

II-Woo Yang (PhD Bartsch 1987) returned to Korea for a faculty position at Korea Military Academy after receiving his PhD. His daughter, Hae Kyung, just completed her PhD from Cornell University and has joined the TTU faculty in the Department of Political Science.

Student News

On April 12, three graduate students in the Department of Chemistry & Biochemistry were announced as winners in the Biochemistry category at the Sixth Annual Graduate Student Research Poster Competition held by the Graduate School at Texas Tech University. First place was awarded to **Simerjeet Gill**, second place to **Yanping Gao**, and third place to **Charlotte Sisk**. All three students are members of Dr. **Louisa Hope-Weeks'** research group.

Chemistry undergraduate student, **Geneva Peterson**, was awarded a National Science Foundation Graduate Fellowship. She has worked primarily with Drs. **Dominick J. Casadonte** and **Louisa J. Hope-Weeks**. Ms. Peterson is a two-year winner of the Goldwater (\$7500/year for undergraduates).

Geneva was also awarded a Gates-Cambridge scholarship. The Gates is used for study at University of Cambridge (UK) for up to 4 years. It is valued at approximately \$160,000. Her award is TTU's fourth Gates-Cambridge award.

Camille Robinson, a junior Biochemistry major, was selected as a finalist in the Harry S. Truman scholarship competition. This scholarship is for \$30,000 toward graduate school for a student intending to pursue a public service career. TTU has only one Scholar and three other finalists on record. She has been admitted to Texas Tech University Health Sciences Center School of Medicine. Camille was working in Dr. **W. David Nes'** lab.

Graduate student, **Cynthe Sims**, received the 2007 Science: It' A Girl Thing (SIGT) Provost Award and fee waiver. These awards are possible due to the generosity of Provost Marcy who for the second year has contributed \$25,000 to IDEAL for SIGT graduate student assistantships. Each recipient is responsible for teaching one SIGT class. Cynthe is a member of Dr. **Robert Shaw's** group.



Dr. **Dominick Casadonte** congratulates **Geneva Peterson** at the American Chemical Society's Awards Banquet.

Jessica McCoury, Cell and Molecular Biology major and

Chemistry minor, received an Outstanding Poster award at the American Chemical Society Southwest Regional Meeting held Nov. 4-7 in Lubbock, TX. Her poster, entitled "Improvement in Sonochemical Efficiency Using Heterodyne Ultrasound", was one of three posters in the general poster session to receive special recognition, and was the only poster prepared by an undergraduate to receive a general session award. Jessica is a member of the Honors College and is an Undergraduate Research Fellow with Dr. **Dominick Casadonte.**

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