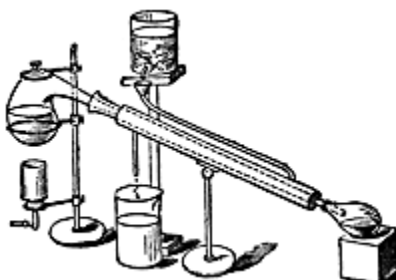




SOUTHWEST RETORT



SIXTY-FOURTH YEAR

APRIL 2012

*Published for the advancement of
Chemists, Chemical Engineers
and Chemistry in this area*

published by

The Dallas-Fort Worth Section, with the cooperation of five other local sections of the American Chemical Society in the Southwest Region.

Vol. 64(7) APRIL 2012

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The Southwest RETORT is published monthly, September through May, by the Dallas-Ft. Worth Section of the American Chemical Society, Inc., for the ACS Sections of the Southwest Region. Contact the Editor for subscription and advertisement information.





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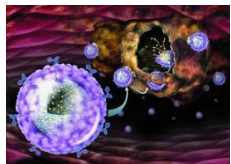
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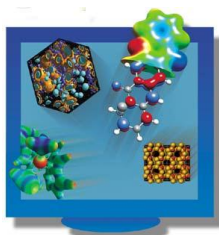
TEXAS EASTMAN

EMPLOYMENT CLEARING HOUSE

Job applicants should send name, email, and phone, along with type of position and geographical area desired; employers may contact job applicants directly. If you have an opening, send your listing, including contact info for your company, to retort@acsdfw.org. Deadlines are the 7th of each month.



Positions Available: Two (2) qualified doctoral level scientists to work on a recently-funded project in nanoscale materials, effective immediately. Due to the nature of the funding source supporting these positions, US citizenship/permanent residency status is required. Interested individuals contact **Jeff Coffey** (j.coffey@tcu.edu) or by phone at (817)257-6223.



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CONTEST!

The DFW Section needs a logo and a slogan of its own, so the section is sponsoring ...with prizes!...a contest for each. Submit entries to retort@acsdfw.org as pdf or jpeg for logo and word format for the slogan.

\$100 prize for each !

**Deadline May 15
Winners will be announced
in the September Retort.**

**NOTE:
May not incorporate or
resemble any part of the
national logo or slogan.**

...AND ANOTHER THING...

DENISE MERKLE, PHD

The variability and plasticity of genetics endows each human with a unique genome - or to be more precise, a genome in which the probability of a completely identical match is vanishingly small. Mutations personalize our genes, and environment modifies us even more. Often it seems that the clichéd blueprint of our DNA has very little impact relative to the changes wrought by the designer nature of external stresses. Take, for example, interpersonal interactions. Any number of societally defined characteristics are encoded in our genetics; genes, or combinations thereof, predispose people to such behaviors as happiness, skepticism, fear and anger. These same traits are also recognizably induced by experiences. Sunny people can be brought to fear and anger by mistreatment. Life-threatening situations can rob risk-takers of their bravery and *joie de vivre*. Cause and effect are both encoded and reactionary, and as a result we all develop different outlooks and personal dogmas.

So, a corollary of this roiling flask of human reagents is that it's not possible to just know what is going to distill over. There's not a defined boiling point for human beings, because the exact composition of the human mixture is immeasurable. People cannot inherently know what others think, what they want, or how they wish to pursue their

lives. Dogmas don't have CAS numbers. This type of information must be revealed by discussion, and discussion is also unique and variable.

Adding everything into the reaction vessel and cranking up the burner isn't a good plan for chemistry; its human counterpart won't work, either. If we actually care about the hidden thoughts of other humans, what should we do?



Guessing is inaccurate, and we all know what happens if we assume communication

is the answer. We must talk. We must initiate the process by acting (if not feeling) respectful of others. Then, calmly, with regard for their right to hold opinions contrary to our own, we must listen to them. Although this is nearly impossible to do, it is the only way to effectively gather data. Our responses should be tempered with the recognition that we, as humans, rely on other humans for a significant portion of the knowledge we amass in life. Agreement is not required, but the ability to say so without offending ought to be.

Currently, the idea of civil discourse seems almost silly. Almost constantly we are bombarded by emphatic assertions that the loudest and most forceful among us are right, and everyone else is wrong. Perhaps what is needed is the acknowledgement that

one person's interpretation is another's Incorrect, and that what we really should have is dialog, not intense subjective rhetoric. Discussion without contention is a path to knowledge. Regardless of whether we agree with each other, it is useful - and intelligent - to know with what one is disagreeing.

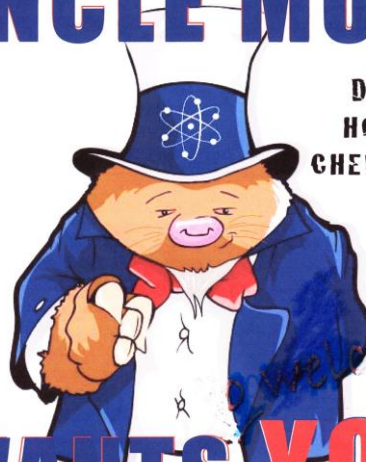
While a little civil communication can lead us to resolution, it can also identify those topics which shouldn't be rehashed at all. It's possible to understand without condoning, and also to reach beyond to the point of agreeing-to-disagree.

Respect, regard, calmness and acknowledgement. Use these tools in the pursuit of effective communication and civil discourse. Will I? Probably not - but you should.



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WATER CAN FLOAT ON OIL

ACS News Service Weekly

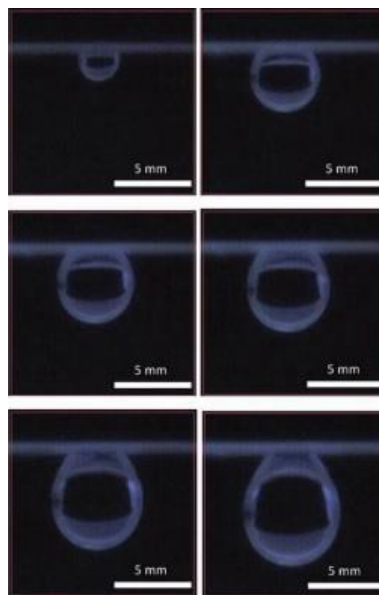
Chi M. Phan*, Benjamin Allen, Luke B. Peters,
Thu N. Le, and Moses O. Tade
Langmuir, **2012**, 28 (10), pp 4609–4613

Defying thousands of years of conventional wisdom, scientists are reporting that it is possible for water to float on oil, a discovery they say has important potential applications in cleaning up oil spills that threaten seashores and fisheries. Chi M. Phan and colleagues point out that the ancient Greek philosopher Aristotle made an early attempt to explain flotation around 350 B.C. Today, most people know that less dense liquids float on more dense liquids. So crude oil with a density of about 58 pounds per cubic foot floats on sea water, which has a density of 64 pounds per cubic foot, and not vice-versa.



Correct?

Phan's team decided to test that notion with computer models and in the lab. They report that in certain cases, the conventional wisdom is wrong. By adding tiny amounts of water to a floating droplet of oil, they found that the ability of water drops to float at the surface of an oil bath depends on both




the size of the droplet and the type of oil.

Commercial vegetable oil has enough surface tension — the force between liquid molecules that allows

beads of water to form or insects to walk on water — at its interfaces with air and water to support a droplet's weight, while pure mineral oils do not. At the same time, they found that vegetable oil could not support drops bigger than about one one-hundredth of a cubic inch. The authors suggest the new knowledge could help clean up oil spills, where water-borne, oil-eating microbes will mix more easily into the oil if suspended in the tiny droplets they describe. "This result can lead to a new and advanced mechanism in processing oil/water mixtures, such as biodegrading process of unwanted oils, including vegetable oils, sand oil tailings and oil spillages," the authors said.

[View a video of their experiment.](#)

22 Ti 47.867	23 V 50.942	24	25	26	27	28	29	30	31	32	33	34 Se 78.96	35 Br 79.904	
40 Zr 91.224	41 Nb 92.906												52 Te 127.60	53 I 126.90
72 Hf 178.49	73 Ta 180.95												84 Po (209)	85 At (210)
104 Rf (261)	105 Db (262)													
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57 La 138.91	58 Ce 140.12	Pt 140.91	Nd 144.24	Pm (145)	Sm 150.36	Eu 151.96	Gd 157.25	Tb 158.93	Dy 162.50	Ho 164.93	Er 167.26	69 Tm 168.93	70 Yb 173.04	



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A COUNCILOR REPORTS

By E. Thomas Strom

I suppose the expected title for a piece like this would be “Council Report.” However, I am one of three councilors for the Dallas-Fort Worth ACS Section, the others being Angela Wilson and Linda Schultz, and they might well emphasize different things entirely. “A Councilor Reports,” I hope, gets the idea across that this is my individual take on things. The point I want to make is that much of the most important activity does not take place in the formal Wednesday Council meeting, but ahead of time.

The ACS Council is something like a legislative body, and like a legislature, a lot of the activity takes place in committee meetings. I am on the Committee on Economic and Professional Affairs (CEPA), and this body meets all day Saturday before the meeting and also on Sunday morning when the ACS meeting officially starts. The CEPA committee has many further obligations, such as monitoring ACS short courses and critiquing new short course presenters. This often spills over into Monday and Tuesday, with the Council meeting following on Wednesday morning.

When I was first elected to Council, one of my fellow D-FW councilors was Urszula Wettermark, who at that time served on CEPA. I felt that CEPA had

to be one of the most important committees, and I wanted to become a member. Urszula introduced me to the then Chair of CEPA, Marinda Wu (current ACS President-Elect), and Marinda graciously let me sit in on all the meetings, even though I wasn’t a member. The following year I was appointed an Associate Member of CEPA, and eventually I became a full member.

CEPA interfaces with ACS staff from the Careers Office. My experience with the staff is that they are very conscientious and sharp! The head of the office is organic chemist Dr. David Harwell, who is just as impressive as any person I have ever met in industry or academia. The ACS tops any other professional organization in the services it provides for members. The ACS is particularly strong in Career Services, yet I fear that many ACS members still don’t realize all the myriad career services that are available.

A lot of the CEPA work is done in subcommittees, so part of the meeting involves those subcommittees. Those subcommittees are Events, Volunteers & Employment Services, Publications and Marketing, Public Policy, and Surveys, plus an additional subcommittee on Standards and Ethics

made up of one representative from each of the other subcommittees. I serve on Publications and Marketing and Standards and Ethics. I was originally on a subcommittee on Professional Services, whose duties included accepting (or not) candidates for Career Consultants, vetting booklets on chemical careers, and choosing outstanding ACS local sections. A reorganization shrank the number of subcommittees by one, so subcommittee tasks were reallocated. One of the important tasks of the Professional Services subcommittee is to brainstorm along with ACS staff ways to get knowledge of the services out to the members. A new ACS services packet had just come out on Mar. 23. I intend to get a large number of those packets in the next couple of weeks, so anyone interested can contact me to get one.

The whole CEPA committee then was informed of the newest job results, which you readers have undoubtedly read about in *C&EN*. The unemployment rate for chemists is now 4.6%, the highest ever in the 40 years that ACS has been measuring such things. Of course, if the overall unemployment rate for the country were 4.6%, we'd all be turning cartwheels, because an unemployment rate of 5% or under used to be considered full employment. However, we chemists are used to a 1% unemployment rate. The only ray of hope was that the changes in chemists'

employment often lag the national average by a year.

A couple of years ago ACS staff and leadership realized that traditional chemists' jobs might not return too quickly. It was thought that small companies were the key to increasing jobs, so ACS started an Entrepreneurial Initiative. An advisory board has been created, and scholarships will be available for entrepreneurial training. There are 50 applicants for the first program, and these range from veteran chemists with 30 years' experience to students still in graduate school.

C&EN is starting a monthly column called ACS Career Tips. The CEPA committee was given four versions by four different authors for the first column, "Five Steps to Successful Networking." A large majority of the committee voted for one version, and that was the version that *C&EN* chose to run. If you look at page 50 of the April 2 issue of *C&EN*, you will see the committee's choice. The only thing I would add to this column is that you do NOT start a network when you learn your job may be in danger; you start your network well before.

It would be tedious for me to go over every action of the CEPA committee, but the main Message is that huge amounts of ACS business are carried out in committee. The most important task of the Council meeting on Wednesday, Mar. 28, was to select two

candidates for ACS President. The ACS President is the visible face of the Society for a year, and you want someone not only bright but also articulate. Those attending the meeting had a chance to hear the candidates at a forum earlier in the week. The four candidates were Thomas J. Barton, Luis A. Echegoyen, William A. Lester, Jr. and Barry M. Trost. All four gave a brief talk to the Council before the vote. The Council then chose Barton from Iowa State and Echegoyen from UT-El Paso as the two candidates. Of course, a petition candidate for President-Elect may surface later in the year.

A special discussion item was “What is your reaction to the proposed topics for the ACS Climate Science Toolkit?”

Prior to the discussion, we were given a set of questions on climate science. We were NOT given the answers. When councilors complained to President Shakhashiri about this, he directed them to the ACS website, a sneaky way to get us to link to the website. There was vigorous discussion on the topic, and it

is clear that ACS councilors are not of one mind about the causes of climate change.

This spring’s Council meeting lacked controversial items, but that doesn’t mean that controversy won’t surface in the future. The point of this piece is that an awful lot goes on before items ever get to Council. On one level the ACS Committees make ACS work, but at another level you members also make ACS work with your volunteering at the local section as well as at the national level. To quote ACS Board Chair Bill Carroll, “We get tremendous sweat equity from our volunteers.” Please keep up the good work.

Preview of coming attractions! I was able to score my eighth interview with an ACS President-Elect. Dr. Marinda Wu gave me a one hour, 15 minute interview. Look for it in a future Southwest **RETORT**.

Remember, the **RETORT is on issuu.com. One good thing about issuu.com is that you can *subscribe* to your publication; if you put in your email (right next to the **RETORT** on the site), you will automatically get the **RETORT** when we post it. (*In order to subscribe, download, or print, you need to register with issuu.com; it’s free and you can opt out of extraneous emails.*) The Retort is still and always will be available on the DFW section’s website acsdw.org. On that site, under *SW Retort*, you can access a pdf (just click on the *name of the month*), a flip-page PC version, and a flip-page MAC version, all of which are downloadable and printable.**

DFW ACS EXTENDS SPECIAL THANKS!!

The *FIRST* ACS DFW Industry and Small Business meeting was held at Dallas Baptist University on March 24th, 2012.

Thank you to all who provided Presentations and Table Hosts:

Abbott	CorsiTech	Ricca Chemical
Ana-Lab	GAF Corporation	SciConsult, Inc.
Arkon Consultants	Mettler-Toledo Inc.	Sovereign Pharmaceuticals
BioBasic USA	Omn Scientific	Terracon
ChK	Reata Pharmaceuticals	TriQuint Semiconductor

DFW ACS's March Industry and Small Business meeting was a great success, with over 90 in attendance and representatives from numerous



companies throughout the section. It was held in DBU's Great Hall. We are especially grateful to National ACS for providing a \$1000 grant to help put on the meeting, which provided companies and individuals a conduit to find potential employees and employers. In addition to the above companies taking the time to share who they are and what they do, many also donated to the local DFW ACS section and collectively raised ~\$2,000 dollars for the local section to sponsor upcoming chemistry education projects and chemistry meetings. I invited the companies to share with me a brief profile about them and have shared those here. Please take the time to read over and support these companies in any way

you can. You may find that the services or products you need are provided by companies right in the DFW section.

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ChK Group Inc. mission is to develop tailored amorphous and nanophase technologies using good science, engineering and environmental principles. The Founder of the company is Dr. Rajan K. Vempati, who has Ph.D. in Soil Chemistry and Mineralogy, Texas A&M University, College Station, and was awarded a prestigious National Research Council, Washington, DC, Junior Postdoctoral Fellowship to research at NASA, Houston, TX. Patented technologies developed are:

- Biosilica blended cement for High Performance Concrete (HPC), and

manufacture of ZSM-5 and Mordenite. See **Manufacture**.

- Filters for removal of As(III) and As(V) from contaminated- and drinking-waters using nanophase Fe oxide coated with zeolite (NpFeZ).
- Multi-nutrient slow release and plant growth medium using NpFeZ for golf green constructions, horticulture and floriculture.
- Stabilization of nanophase Mn(VII) oxide on natural and synthetic solid supports and fabrics, and its applications. A few applications are:
 - Degradation of chemical and biological warfare agents using non-woven fabrics.
 - Easy and rapid synthesis of disulfide using different thiols and Friedel-Crafts reactions.
 - Odor control N and S based compounds.
 - Biocide and algacide with and without fabrics.
 - Degradation of quaternary ammonium compounds.

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TriQuint provides innovative RF solutions for mobile devices such as smartphones and tablets, as well as the global networks that transport voice, data and video communications. The company experienced its sixth consecutive year of record revenue in 2011, and was named to Fortune[†] magazine's annual 100 Fastest-Growing Companies list. Additionally, TriQuint has been on the *Business Journal's* "Most Admired Company" list in the Oregon technology category the last four years. Visit our website at <http://www.triquint.com> for more information.

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SciConsult Inc. provides diverse, project-based consulting services, including but not limited to project planning, such as complete protein or peptide characterization plans; troubleshooting of experiments, assays and/or projects; requirement assessment for facilities and laboratories; collaboration development and maintenance, and grant writing and editing.

Arkon Consultants specializes in industrial cleaners and surface treatments, reformulations, troubleshooting, and new formulations for specialty cleaning.

AROUND-THE-AREA

UTA

DASGUPTA WINS 2012 DAL

NOGARE AWARD: UTA Jenkins
Garrett Professor **Purnendu “Sandy”**



Dasgupta was honored Mar. 12 at the Pittcon Conference in Orlando as the winner of the Del Nagare Award. This award, given by the Chromatography

Forum of the Delaware Valley since 1972, honors scientists for their contributions to the understanding of the chromatographic process. Sandy has made numerous improvements to the methods of ion chromatography. He is credited with the development of electro-dialytic suppressors, eluent generators, and post column reagent introduction devices.

SHIMADZU ADVANCED ANALYTICAL CENTER OPENS

AT UTA: April 9 marked the opening of the Shimadzu Center for Advanced Analytical Chemistry in the UT-Arlington (UTA) Chemistry and Physics Building. UTA President **James D. Spaniola** gave remarks at the 3:30 p.m. ribbon-cutting ceremony, which was followed by remarks from top Shimadzu executives visiting from Japan. The equipment donations from Shimadzu are valued at \$3 million, and the Center contains \$6 million worth of state-of-the-art chromatography, mass spectrometry, and spectroscopy equipment. This is one of the biggest

gifts ever given to the UTA College of Science, and UTA is now the site of the biggest concentration of Shimadzu instruments in the Western Hemisphere. In addition, Shimadzu has endowed the Shimadzu Distinguished Professorship of Analytical Chemistry.



The center director, Associate Professor of Chemistry **Kevin Schug**, will be the holder of this endowed

chair. Besides its use by UTA research faculty, the facility will also be available for use by area businesses on a contract basis.

Dr. Rasika Dias gave an invited talk on “Nitrogen Based Ligands in Gold Carbonyl, Alkene, and Alkyne Chemistry” at the San Diego ACS meeting as part of the awards symposium honoring Dr. **Philip P. Power** of UC-Davis, winner of the 2012 ACS Award in Organometallic Chemistry. Some of the gold-alkyne work by Dr. Dias and his coworkers was recently reported in *Angewandte Chemie International Edition*.

Dr. Frederick M. MacDonnell gave an invited talk at San Diego on “Redox-Active Ruthenium(II) Polypyridyl Complexes at Potential Anti-Cancer Drugs with a Hypoxia Sensitizing Mechanism,” with coauthors **Sanjay Awasthi, Abhishek Yadav, Thamar K. Janaratne, Sharad S. Singhal, Cynthia A. Griffith, and Yanglin**

Chen. Another oral presentation from the Macdonnell group was given by **Steven Poteet** with coauthors **Cynthia Griffith, Dr. Shreeyukta Singh, Dr. Zachary Breiback, Dr. Daniel Armstrong,** and **Dr. Macdonnell.** In addition, there were four posters from the group with additional coauthors **David Boston, Kai-Ling Huang, Norma Tacconi, Reynaldo O. Lezna, Maher D. Rashdan, Brian H. Dennis, Ying Zhang,** and **Kenneth Abayan.** Professor **Krishnan Rajeshwar** has moved from the position of Associate Dean of Science to that of Associate Vice President for Research. Two recent special seminars were given by Dr. **Joachim Weiss** on “Modern Ion Chromatography, Principles and Applications,” Mar. 29, and Dr. **Jianhua Wang** on “DNA Extractions by Ionic Liquids,” April 2.

BAYLOR

Dr. **David E. Pennington**, Professor of Inorganic Chemistry at Baylor since 1969, received his 50-Year ACS Membership Pin in late February. Dr. **Sung-Joon Kim** joined Baylor in Fall 2011 from a PhD and postdoc at Washington University. He will study the composition and structures of complex biological solids. Dr. **Touradj Solouki** (PhD Texas A&M) also joined us from the University of Maine (Orono campus) this past fall. Touradj studies x-omics using ICR-mass spectrometry and ion mobility. And for fall 2012 we have hired Dr. **Kevin Shuford** (PhD Univ of Florida) away from Drexel

University. Kevin specializes in theoretical chemistry of interest in chemistry, physics, materials science and engineering.

UD

Dr. **Scott Boegeman** and Dr. **Ellen Steinmiller** attended the Spring ACS meeting in San Diego, along with several students: **Michelle Baalman, Rachel Yuengert, Claire McDonogh, Kaylee Gund, Stephanie Ossowski,** and **Anna Marie DeLaRosa.** **Ossowski** and **DeLaRosa** presented poster sessions. **Anna Maria DeLaRosa**, who will be attending graduate school at Texas A&M, received an honorable mention for a NSF Graduate Research Fellowship. She is a 2011 recipient of a Goldwater scholarship; **Justin Samorajski** was a runner-up.

TCU



National Chemistry Week 2012

TCU Chemistry Club will be again working with the Fort Worth Museum of Science and History, spearheading National Chemistry Week! Last year's event brought in over 4,000 guests and over 120 volunteers! If you're interested in participating for Fall 2012, please contact TCU Chemistry Club at [**chemistryclub@tcu.edu**](mailto:chemistryclub@tcu.edu).

TARLETON

Peter Bell, Linda Schultz, and Lance Whaley attended the San Diego National Meeting with 3 undergraduate students, each of whom presented research posters. The Tarleton Student Affiliate Chapter received recognition as an *Outstanding Chapter* and also won a student chapter *Green Chemistry Award*. ACS Student Chapters are recognized as Green Chemistry Chapters by engaging in at least three green chemistry activities during the academic year. ([Click here for more information.](#))

TEXAS TECH

On March 28, 2012, **Edward Quitevis**, Professor in the Department of Chemistry & Biochemistry, gave an invited presentation entitled "Optical Kerr Effect Spectroscopy and Molecular Dynamics Simulations of Nonpolar and Polar Molecules in Ionic Liquids" at the 243rd American Chemical Society National Meeting in San Diego, CA.



UTD

The UT Dallas Chemistry Department welcomes a new colleague, Dr. **Bruce M. Novak**, former head of the Department of Chemistry at North Carolina State University, who will also serve as the Dean of the School of Natural Sciences and Mathematics.

Born in Flint, Mich., and raised in Southern California, Novak joined the U.S. Army for a five-year stint before enrolling at The California State University at Northridge, where he graduated summa cum laude in 1983 and obtained his master's degree in chemistry in 1985. Novak earned his doctoral degree from the California Institute of Technology in 1989.

Novak began his academic career at the University of California at Berkeley, where he earned a DuPont Young Investigator Award twice, an Alfred P. Sloan Research



Fellowship, a National Science Foundation Presidential Young Investigator Award, and a NSF Presidential Faculty Fellowship. He accepted a position in 1993 at The University of Massachusetts at Amherst in the Department of Polymer Science and Engineering before moving in 1998 to North Carolina State University, where he was a Distinguished University Professor. During his time at UMass, Novak was awarded the NSF Carl S. Marvel Creative Polymer Chemistry Award.

Novak's polymer research program currently encompasses projects in several major areas in materials chemistry, including macromolecular chirality, optical switches, and molecular machines. Although he

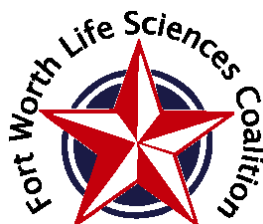
excelled in research, Novak says teaching has always remained a great passion. “There are few times in life where you can truly have an impact on someone, and I find teaching to be an incredibly rewarding experience. I believe very strongly in the university system. Over the last millennium, modern universities have played a pivotal role in the progress of human understanding of the world around us.”

MEETINGS

ISSF 2012 (10th International Symposium on Supercritical Fluids) will be held May 13-16 in San Francisco. More information and registration can be found at **ISSF2012.com**.

ACT₂ Biennial Conference

June 24-28, 2012 at the University of Mary Hardin Baylor
<https://sites.google.com/site/act2tx>



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*Some of the world's greatest feats were accomplished by people not smart
enough to know they were impossible....*

Doug Larson

PINE NUT WHAT?

New study of pine nuts leaves mystery of “pine mouth” unsolved



Characterization of Pine Nuts in the U.S. Market, Including Those Associated with “Pine Mouth”, by GC-FID. Ali Reza Fardin-Kia, Sara M. Handy, and Jeanne I. Rader. *J. Agric. Food Chem.*, **2012**, 60 (10), pp 2701–2711

A new study of the composition of pine nuts, including those associated with “pine mouth,” leaves unsolved the decade-old mystery of why thousands of people around the world have experienced disturbances in taste after eating pine nuts. The report on pine nuts or pignolia — delicious edible nuts from pine trees enjoyed plain or added to foods ranging from pasta to cookies — appears in *Journal of Agricultural & Food Chemistry*. Ali Reza Fardin-Kia, Sara M. Handy and Jeanne I. Rader note that more than 20,000 tons of pine nuts are produced each year worldwide. “Pine mouth,” first reported in Belgium

in 2000, is a bitter metallic taste that develops within one to two days of

eating pine nuts and can last from one to two weeks. In 2009, the French Food Safety Administration reported a possible link between “pine mouth” and consumption of nuts of *Pinus armandii*, a pine species whose nuts are not traditionally eaten by humans.

Researchers have identified certain fatty acids whose levels vary among pine species, making them a potentially useful tool for telling different species apart. To determine the source of pine nuts sold in the U.S.--the first such effort--they measured the ratio of these compounds to the overall amount of



fatty acids in the nuts.

Using fatty acid composition and a fatty acid

diagnostic index (DI) along with DNA analysis, they found that most pine nuts sold in the U.S. are mixtures of nuts from different pine species, including *Pinus armandii*. They report that combining the fatty acid DI and DNA analysis is a useful way to determine which samples of pine nuts are mixtures of nuts from several species, but that this information itself may not definitively predict which pine nuts may cause “pine mouth.” Its cause remains a mystery.

FIVE QUESTIONS FOR.....

Our April volunteer is Mr. **Steven Twaddle**, MS, a Materials Engineer in Non-Metallic Materials for Lockheed Martin Aeronautics in Fort Worth, TX.

ACS Activity: Member, Awards Committee of the DFW Local Section

1) How old were you when you realized you wanted to be a scientist?

16

2) What was your first job in science? Did you like it?

Analytical chemist doing failure investigation of rocket parts; I liked it because I learned a lot about a wide variety of materials.



3) What do you enjoy about your current job?

Resolving complex technical issues on the F-35 fighter.

4) What would you change about chemistry in the US, if you could?

Exposing children to the fun of

chemistry at younger ages.



6) What was your most memorable experience in science?

My "15 minutes of fame" was when, by proxy, my finger was in the Secretary of the Navy's ear. I helped develop processes for the manufacture of individualized ear pieces to be used on-board the flight deck of aircraft carriers. The first articles were for the Secretary of the Navy.

Thank you, Mr. Twaddle, for your interesting remarks! To volunteer to be interviewed, e-mail to retort@acsdfw.org.





PRINT AND POST !

APRIL 2012
The Dallas Fort-Worth Section
of
The American Chemical Society
presents the
45TH ANNUAL MEETING-IN-MINIATURE

University of Dallas
Saturday, April 21, 2012
8:00 am to 4:30 pm
Gorman Lecture Center



Format: 15 min. talks
Categories: Undergraduate Students and
Graduate Students

**For the first time, the Meeting-in-Miniature schedule and
abstracts are in the Southwest RETORT!**
Schedule: pages 25-27 Abstracts: pages 28-58

For more information, contact: Bill Hendrickson at
hendrick@udallas.edu

Each presentation should be carefully planned for effective delivery in 15 minutes. This will be followed by an ~5 minute question, answer, and discussion period with your audience. Here is a set of guidelines (Ten Simple Rules for Making Good Oral Presentations) to keep in mind as you are preparing your presentation:

<http://www.ploscompbiol.org/article/info:doi/10.1371/journal.pcbi.0030077>

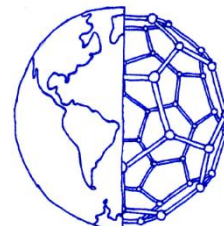


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ACT₂ BIENNIAL CONFERENCE

Chemistry Makes the World Go Round



When: June 24-28, 2012

Where: The University of Baylor Mary Hardin in Belton, TX
(173 miles from Houston, 140 miles from Dallas, 61 miles from Austin, 140 miles from San Antonio)

Cost: \$250 (early bird pricing until May 25th) includes registration, all meals from Sunday night through breakfast Thursday, and lodging from Sunday night until Thursday (or \$125 for registration and all meals except breakfast-no lodging) **
Presenters save \$50 off the above prices!!!

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1. Get all of your Professional Development hours for the year!
2. The lowest cost chemistry conference you will find anywhere!
3. The University of Mary Hardin Baylor is a small beautiful campus with **FREE PARKING!**
4. Many workshops covering all levels of chemistry, from your lowest academic students to your brightest AP students!
5. It will be 5 days of Chemistry Fun!
6. Gets tons of ideas to implement in your classroom!
7. Door Prizes: everyone will win something!
8. Come see old friends and meet lots of new friends for networking!
9. World-renowned presenters Robert Becker and Ken Lyle!
10. Demos in the Dark: all the demos you can't do inside because they are too big or dangerous (you won't want to miss this)!

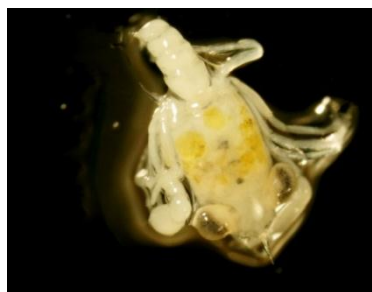
For more info and to register:

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Click link at bottom of webpage to register and/or present

From the editor:

How do I pick the articles from the ACS Press Room every month? Well, I liked the pine nut article, but it was because my son says *he* has pine nut mouth...I thought he was making it up or razzing me. The oil droplet article?...Now, as a surfactant chemist, I really don't care which floats on which...I just want them to *coexist* in a nice, stable emulsion and act like a solution. In fact, there are oils which do sink in water—for example, brominated oils used in metalworking sink like a rock, and are the very devil to emulsify. I began to hunt on the internet for other instances of high density oils and the like, and as usual found several things which caught my attention. Much of the oil lost in the BP oil spill did emulsify with natural contaminants in water; some fractions sank, contaminating silt and bottom feeders, and some ended up in rather unlikely places. The photos are of blue crab larvae with oil trapped inside their shells, souvenir of the oil spill. The blue crab (food for many natural predators) is



considered to be a primary indicator of the health of the ecosystem of the Gulf (full article on nola.com), and no one can think this is a good sign, least of all Harriet Perry, director of the Center for Fisheries Research and Development at the Gulf Coast Research Laboratory (GCRL).

Where did the larvae come in contact with these oil micro-droplets at the critical shell-forming phase of their development? Perry says the crabs spawn near shore in marshes, and the tiny larvae head out to sea and pass through several stages before returning to settle along the coast. In the marshes, waters that were heavily impacted by the oil spill, larvae are in contact with and did pick up dispersed oil droplets beneath their shell. Researchers hope the oil droplets will be shed as larvae develop and molt. The dispersed droplets must be located throughout the levels of water, neither floating nor sinking. Is the oil emulsified (doesn't appear to be)? Do the droplets adhere to very small particles of silt, keeping them drifting at levels not usually occupied by oils...how have the droplet densities been altered? Are, as suggested by the article on page 7, tinier droplets of water added to tiny oil droplets? So many questions...never enough time!

The 2012 Meeting-in-Miniature is scheduled for April 21; the schedule and abstracts are included in this issue. Look for the winners in the May issue!

Best regards,



Meeting in Miniature 2012 Schedule

No.	Time	Name	Graduate A School	Gorman A Advisor
G01	8:45	Bishnu Subedi	UTA	Pierce
		Biophysical characterization of MiaE: an unusual non-heme diiron hydroxylase involved in tRNA post-transcriptional modification		
G02	9:00	Andra Carter	UTA	Pierce
		Development of small substrate surrogates for mechanistic and spectroscopic characterization of the O ₂ -dependent tRNA modifying Mia.		
G03	9:15	Margarita DeJesus	TWU	Anderson
		Protein-protein interactions at the interface of human glutathione synthetase		
G04	9:30	Alysia Lowe	UTD	Balkus
		Acrylonitrile-based fibers for enhanced wound healing with nitric oxide		
G05	9:45	Anne Marti	UTD	Balkus
		Silver-functionalized [Zn ₂ (bpdC) ₂ (bpee)] films: a luminescent metal organic framework for the detection of ethylene		
G06	10:00	Nimanka Panapitiya	UTD	Ferraris
		Fabrication and characterization of novel metal organic framework stabilized immiscible polymer blend membranes for gas separation		
	10:15	Break		
G07	10:30	Jing Lui	UTD	Musselman
		Spin-coated mixed-matrix membrane for gas separation at high pressure and high temperature		
G08	10:45	Fadwa Anka	UTD	Balkus
		Formation of gold nanoparticles in situ while electrospinning a polymer/Au ³⁺ solution under uv light		
G09	11:00	Jeliza Bonzo	UTD	Ferraris
		Carbon nanofibers from electrospun PAN/6FDA-NDA as electrodes for electrochemical double-layer capacitors		
G10	11:15	Sumudu Wijenayake	UTD	Ferraris
		Asymmetric mixed matrix membranes fabricated using a spin coating technique		
G11	11:30	Daniel Tran	UTD	Balkus
		Electrospun core-shell Nafion/enzyme membranes for biofuel production		
G12	11:45	Udayana Ranatunga	UTD	Nielson
		Utilization of continuum models for nanosolids in soft matter environments		
	12:00	Lunch		
G13	1:30	Andrew Mahler	UNT	Wilson
		Reduced computational costs in the correlation consistent Composite Approach (ccCA) through explicitly correlated methods		
G14	1:45	Matthew Carlson	UNT	Wilson
		Determination of equilibrium geometries using ccCA energy gradients		
G15	2:00	Amanda Riojas	UNT	Wilson
		Development of a solvated composite method: The Solvated correlation consistent Composite Approach (Solv-ccCA)		

G16	2:15	David Bushdiecker	UTD	Musselman	The effect of carboxylic acid functionality on single-walled carbon nanotube cytotoxicity
G17	2:30	Dinushi Samarajeewa	UTD	Musselman	Surfactant peptide/single-walled carbon nanotube (SWCNT) composites with altered electronic properties
G18	2:45	Blake Wilson	UTD	Nielson	A molecular dynamics investigation of single walled carbon nanotube dispersion by surfactant peptides
	3:30	Award Presentation Gorman Faculty Lounge			

Graduate B Gorman B

G19	8:45	Josh Gibson	UNT	Wilson	A titanium potential using the multi-state modified embedded atom method
G20	9:00	Kameron Jorgensen	UNT	Wilson	Recovery of correlation energy via local ab initio methods
G21	9:15	Christopher South	UNT	Wilson	Utility of MR-ccCA in reproducing potential energy curves and constants of diatomic molecules containing third-row elements
G22	9:30	Shirangi Fernando	UTD	Sherry	Breaking the slow water exchange barrier in the design of functional PARACEST agents for MRI
G23	9:45	Leila Fidelino	UTD	Sherry	A New PARACEST agent for the detection and imaging of hydrogen peroxide
G24	10:00	Marie Laury	UNT	Wilson	Density Functional Theory (DFT) for transition metal thermochemistry
	10:15	Break			
G25	10:30	Rebecca Weber	UNT	Wilson	Rearrangement of diphosphine ligands in triosmium clusters: A computational study
G26	10:45	Cong Lui	UNT	Wilson	Computational studies of CO ₂ activation using transition metal catalysts
G27	11:00	Venkata Adiraju	UTA	Dias	Interactions of copper(I)-ethylene complexes supported by 1,3,5-triazapentadienyl ligands containing nitro group
G28	11:15	Naleen Jayaratna	UTA	Dias	Synthesis and characterization of multinuclear Ag(I) complexes possessing argentophilic interaction
G29	11:30	Shannon Woodruff	SMU	Tsarevsky	Synthesis of well-defined polymers with epoxide groups by atom transfer radical polymerization and their use as precursors of functional materials
G30	11:45	Hongzhang Han	SMU	Tsarevsky	Applications of exchange reactions at hypervalent iodine centers for the synthesis of polymeric materials
	12:00	Lunch			
G31	1:30	Sajani Basnayake	UTD	Balkus	Synthesis of novel zeolitic imidazolate frameworks

G32	1:45	Jiaqi Wang	UNT	Wilson	Transition Metal Catalyzed Oxidative Cleavage of C β -O Bond in β -O-4 Linkage of Lignin
G33	2:00	Sanjaya Perera	UTD	Balkus	Hydrothermal synthesis of Graphene-TiO ₂ nanotube composites with enhanced photocatalytic activity
G34	2:15	Anjalee Liyanage	UTD	Balkus	Nanocomposites for photocatalytic applications
G35	2:30	Ting Zhou	TA&MC	Jang	Selective hydrogenation of acetylene over Pd on ionic liquid loaded SiO ₂ support
G36	2:45	Nathaniel Hanson	TA&MC	Jang	Heterogeneous catalysis of Bio-diesel using starch based catalysts under experimental application of ultrasound
	3:00	Minh Nguyen	UTD	Balkus	Conjugated aromatic PPI: Characterization of structure, electronic spectra, and thin films from soluble complexes
	3:30	Award Presentation Gorman Faculty Lounge			

Undergraduate Science Building 114

U01	8:45	Triet Nguyen	UTD	Nielson	Design modifications of SWCNT-dispersing peptides: A molecular dynamics approach
U02	9:00	Josin Kalathil	UTD	Balkus	Synthesis of "Gray" TiO ₂ nanotubes and their photocatalytic activity
U03	9:15	Elaine Chien	UTD	Sherry	Electrospun polyacrylonitrile/ZIF-8 nanofibers as supercapacitor electrode materials
U04	9:30	Hiulam Kam	UTD	Balkus	Mesoporous carbon fibers via electrospinning for supercapacitors
U05	9:45	Tracy Rosales	UTD	Balkus	Mesoporous carbon fibers via electrospinning for supercapacitors
U06	10:00	Bao Nguyen	UTD	Ferraris	6FDA-based polyimides mixed-matrix membranes (MMMs) for gas separations
10:15 Break					
U07	10:30	Jonathan Tsao	UTD	Balkas	Ag ₂ S quantum dot decorated TiO ₂ nanotubes for photocatalytic degradation of organic dyes
U08	10:45	Khiem Vu	UTD	Balkas	Synthesis of reduced graphene/TiO ₂ nanotubes with attached CuS quantum dots
U09	11:00	Do Nguyen	UTD	Ferraris	Novel metal organic framework stabilized immiscible polymer blend membranes for gas separation
U10	11:15	Layne McBeath	UTD	Balkus	The growth of microporous metal organic framework RPM-3 on a laser ablated substrate for olefin detection
U11	11:30	Nigel Gwini	ACU	Powell	New triosmium clusters with two bridging ligands
U12	11:45	Eyerusalem Mamo	UTD	Balkus	Electrospinning hollow chitosan fibers for enzyme immobilization
	12:00	Lunch			

U13	1:30	Anh Vu	UTD	Balkus	Synthesis and characterization of zeolites and metal organic frameworks
U14	1:45	Sabin Kshattray	UTD	Sherry	Translating the power of tcaSIM, a program that simulates isotopomer analysis-based intermediary metabolism, into a graphical interface
U15	2:00	Kimberly Mendoza	SMU	Biehl	Synthesis of biologically important novel pyridobenzimidazoles attached to indole or benzo[b]thiophene structures
U16	2:15	Michelle Baalman	UD	Hendrickson	Mechanism for the highly regioselective chlorination of anisole with household bleach
U17	2:30	James Wheeler	TA&MC	Jang	Selective hydrogenation of acetylene in ethylene over Au catalysts
U18	2:45	Holland Korbitz	Baylor	Garner	Synthesis of pyridinium salts with possible biological activity
U19	3:00	Ruperto Mariano	UTD	Balkus	Reduced graphene oxide- TiO ₂ nanotube composites for use as high-performance photocatalysts
	3:30	Award Presentation Gorman Faculty Lounge			

Undergraduate Student Session
Science Building 114
Chairs : Ms. Anna Marie DeLaRosa
Ms. Claire McDonough

U01 Design modifications of SWCNT-dispersing peptides: A molecular dynamics approach
Triet S.Nguyen (*Tsn101020@utdallas.edu*) and **Dr. Steven O. Nielsen**, *The University of Texas at Dallas, Richardson, TX*

Among the non-covalent schemes of functionalizing and solubilizing single-walled carbon nanotubes (SWCNTs) in aqueous systems, the use of reversible cyclic peptides (RCPs) has emerged as a promising platform for biotechnological applications. Their unique features make them not only an ideal SWCNT-dispersing agent but also a versatile biomolecule carrier. We propose structural modifications to the original RCP design for improving their function by incorporating m-aminobenzoic acid (MABA) units. Here we present our analysis of different energetic aspects of these modified molecules in their interactions with SWCNTs using all-atomistic molecular dynamics simulations.



U02 Synthesis of “Gray” TiO₂ nanotubes and their photocatalytic activity
Josin Sebastian Kalathil (*jsk073000@utdallas.edu*) and **Kenneth J. Balkus**, *University of Texas at Dallas, Richardson, TX*

Our original purpose was to test to see if the grey TNTs had a better photocatalytic activity than the white TNTs and also characterize the grey TNTs using IR. TEM analysis, shown in Figure 1, of the gray TNTs showed that there was a thin layer of what looks like amorphous material on the surface and EDAX did not show anything other than TiO₂. Thus it would appear that the TNT surface had become disordered. The grey TNTs have been shown to have greater photocatalytic activity compared to white TNTs. Our tests showed that for the photodegradation of malachite green and methylene blue, the gray TNTs were significantly more active than the white TNTs as shown in Figure 3. Through these results we can conclude that the grey TNTs do in fact have a better catalytic activity than the white TNTs.

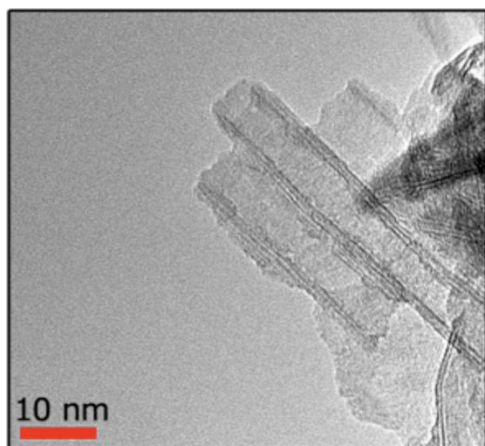


Figure 1. TEM image of gray TNTs

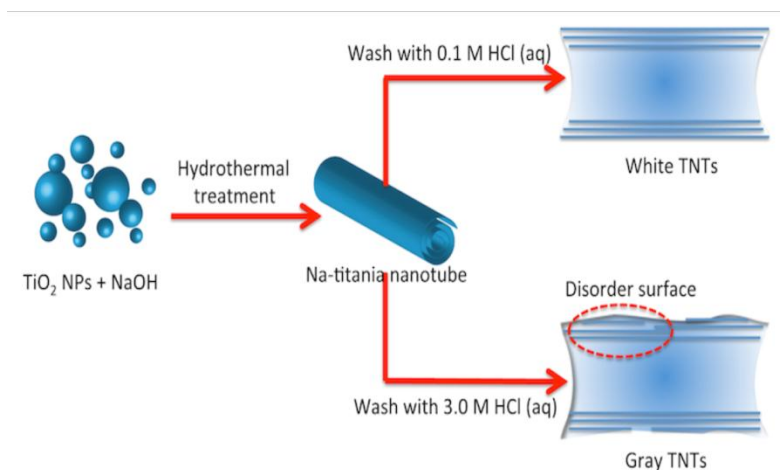


Figure 2. Synthesis of gray TNTs

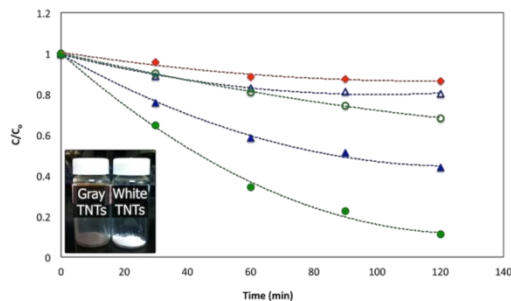


Figure 3. Plot of dye concentration via time for the photodegradation of malachite green by gray and white TNTs.



U03 Electrospun polyacrylonitrile/ZIF-8 nanofibers as supercapacitor electrode materials

Elaine Chien (scx085100@utdallas.edu), Jeliza S. Bonso, and John P. Ferraris, Department of Chemistry and the Alan G. MacDiarmid Nanotech Institute, University of Texas at Dallas, Richardson, TX 75080

Polyacrylonitrile (PAN) is a good carbon source in generating carbon fibers that can be used as electrode materials for supercapacitors. However, its poor porosity limits its electrochemical performance. In order to increase the surface area, PAN-based carbon fibers are incorporated with different materials such as sacrificial polymers, pore-forming agents, and metal organic frameworks (MOF). ZIF-8 [Zn(MeIM)₂; MeIM = 2-methylimidazole], a highly porous zeolite-type of MOF, is suitable as a template for porous carbon synthesis. In this study ZIF-8 was incorporated to PAN and the mixture was electrospun to generate free-standing carbon fibers. PAN/ZIF-8 carbon fibers were able to increase the electrochemical performance of supercapacitor devices with specific capacitance of 96 F/g and energy and power densities of 58 Wh/kg and 1729 W/kg, respectively.



U04 Mesoporous carbon fibers via electrospinning for supercapacitors

Hiulam Kam (hxx093020@utdallas.edu), Daniel N. Tran, Sanjaya D. Perera, and Kenneth J. Balkus, Jr., The University of Texas at Dallas, Richardson, TX

Mesoporous carbon molecular sieves are well-known for their high surface area and high graphene content that is important for conductivity, making them ideal for supercapacitors. Unfortunately, mesoporous carbon sieves are generally made in a powder form. In order to be used in a coin cell type supercapacitor, a binder must be added, which lowers its capacitance. We hereby propose a novel method of preparing mesoporous carbon in a paper form using a technique called electrospinning, which allows a liquid precursor to be “spun” into solid fibers. Using this technique, we can prepare thin sheets of mesoporous carbon nanofibers that can be easily handled, hence doing away with the need for a binder. SEM images showed that the carbonized fibers maintained its morphology, and Raman spectroscopy confirmed the presence of sp² hybridized graphene sheets. Preliminary results for the fabrication and testing of coin cell type supercapacitor devices will also be presented.



U05 Fabrication of hollow polystyrene nanofibers via electrospinning

Tracy Rosales (tir072000@utdallas.edu) and **Kenneth Balkus Jr.**, University of Texas at Dallas Richardson, TX 75080

Electrospinning has become a popular method over the recent years for producing nanofibers easily and at low costs. In this study, polystyrene, an inexpensive, spinnable polymer, was concentrically spun with various solvents, including 1M KCl, 0.1M PBS, and 95% NMP/water, to produce hollow fibers. Hollow fibers (HF) were successfully produced from spinning 25% w/v polystyrene in chloroform with 95% NMP/water, and HF fibers were modified through a sulfonation reaction with sulfuric acid. Modified hollow fibers are useful in numerous applications, such as chiral separation, ion exchange, gas separations, and enzyme immobilization.



U06 6FDA-based polyimides mixed-matrix membranes (MMMs) for gas separations

Bao L. Nguyen (bln100020@utdallas.edu), **Grace D. Kalaw**, **Inga H. Musselman**, **Kenneth J. Balkus, Jr.**, and **John P. Ferraris**, Department of Chemistry and the Alan G. MacDiarmid Nanotech Institute, University of Texas at Dallas, Richardson, TX 75080

Mixed-matrix membranes (MMMs) composed of highly selective zeolitic imidazolate framework (ZIF) nanocrystals and thermally stable polyimides are promising for gas separations. MMMs combine the advantages of the ZIF's superior separation performance and the polymer's processability. To obtain a good interfacial interaction between polymer and ZIF additive, we incorporated a ZIF bearing an aldehyde group (ZIF-90) into hexafluoropropanediamide (6FDA)-based polymers up to 35 wt%. The aldehyde group in ZIF-90 may encourage interactions with the polymer backbone, and with its small pore size (3.5 Å), improvements in permeability as well as selectivity can be achieved. The high molecular weight (>80 kDa) 6FDA-based polyimides, including 6FDA-NDA (2,5-naphthalenediamine), 6FDA-ODA (4,4'-diphenyleneoxide), and copolymer 6FDA-ODA-NDA were used as polymer matrices. The interaction between ZIF-90 and polymer was clearly shown in the infrared (IR) spectra by the shift of the carbonyl peak of ZIF-90 in the MMM. SEM images of the MMM cross-sections also show good contact between ZIF and polymer by the formation of polymer veins around the additive crystals. X-ray diffraction (XRD) studies of the MMMs show that the ZIF-90 crystallinity remains intact in the polymer. Permeability studies for these MMMs are currently being measured.



U07 Ag₂S quantum dot decorated TiO₂ nanotubes for photocatalytic degradation of organic dyes

Jonathan Tsao (jxt075100@utdallas.edu) and **Kenneth J. Balkus, Jr.**, *The University of Texas at Dallas, Richardson, TX*

TiO₂ nanotubes (TNTs) were synthesized via a hydrothermal process. The TNTs were then coated with a bifunctional linker then doped with AgNO₃ and Na₂S solutions to form Ag₂S quantum dots. The TNTs with Ag₂S quantum dots (Ag₂S QDs) were then characterized using FT-IR, X-ray diffraction, UV-vis and transmission electron microscopy. The Ag₂S QDs were found to be around 3-15 nm in diameter. These TNTs with Ag₂S QDs were tested for their photocatalytic activity through the photodegradation of malachite green and methylene blue. The same procedure to create Ag₂S QDs was also followed to create Ag QDs, with diameters between 10-20 nm. The TNTs with Ag QDs were also tested for their photocatalytic activity.



U08 Synthesis of reduced graphene/TiO₂ nanotubes with attached CuS quantum dots

Khiem T. Vu (ktv071000@utdallas.edu), **Sanjaya D. Perera**, **Ruperto G. Mariano**, **Nijem Nour**, **Oliver Seitz**, **Yves Chabal** and **Kenneth J. Balkus Jr.** *The University of Texas at Dallas, Richardson, TX*

TiO₂ is widely used as a photocatalyst under UV light, but is limited by two issues: large band gap and rapid electron-hole recombination. In the current study, TiO₂ nanotubes (TNTs) are synthesized on a reduced graphene oxide support (hGO) through a hydrothermal process. CuS quantum dots were then attached to the inside and outside surfaces. The hGO and CuS QDs are expected to increase charge separation and expand TiO₂'s absorption spectrum to include more of the solar spectrum, respectively. We have prepared hGO-TiO₂ nanotube composites and decorated with CuS quantum dots (Figure 1). The photocatalytic activity of hGO/CuS/TiO₂ nanotubes will be tested for the photodegradation of malachite green, with the rate of degradation monitored by UV-Vis spectroscopy.

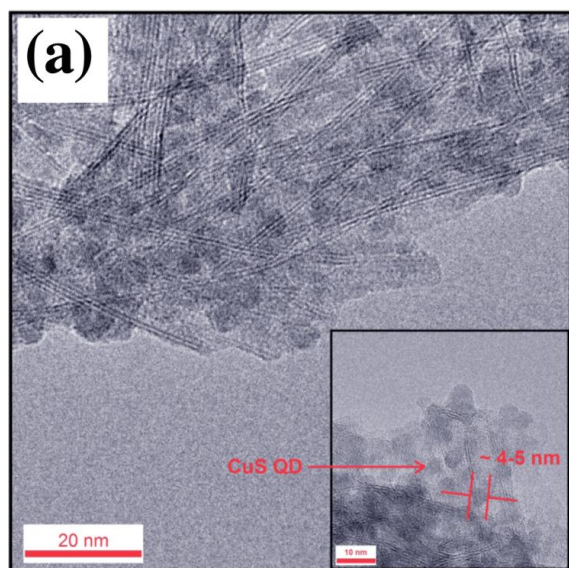


Figure 1. TEM image of hGO-TNTs decorated with CuS quantum dots



U09 Novel metal organic framework stabilized immiscible polymer blend membranes for gas separation

Do D. Nguyen (do.nguyen@utdallas.edu) and **John P. Ferraris**, *University of Texas at Dallas, Richardson, TX*

Polymer blending can be used to enhance the gas separation properties of Mixed Matrix Membranes (MMMs). MMMs combine the mechanical properties of the polymers with the gas separation properties of inorganic porous materials such as metal organic frameworks (MOFs). Controllable blending of a highly permeable polymer with a highly selective polymer for a particular gas pair has shown to enhance gas separation properties. However, due to the inherent incompatibility of most polymers, polymer blending can lead to non-uniform phase separation and surface roughness leading to inconsistent gas separation properties. In order to stabilize phase separated polymer blends, nanoparticles have been used as a compatibilizer for various applications. This approach leads to the formation of more uniform microstructures with reduced film roughness which is beneficial for gas separation membranes. A novel class of MMMs was fabricated by incorporating MOFs in an immiscible polymer blend matrix and the amount of MOFs was varied to enhance gas separation properties. One important advantage of this system is the dual functioning of MOFs as a molecular sieve as well as a compatibilizer. Fabrication and characterization of this novel class of MMMs for gas separations will be presented.



U10 The growth of microporous metal organic framework RPM-3 on a laser ablated substrate for olefin detection

Layne McBeath (ldm076000@utdallas.edu) and **Kenneth J. Balkus Jr.**, *Department of Chemistry, University of Texas at Dallas, Richardson, TX 75080*

Ethylene is a colorless gas that is not only produced in nature but also used in many forms of industry. In recent years, different methods of ethylene detection have been investigated for applications in plant cultivation and agriculture. In this study, a Metal Organic Framework (MOF) called $\text{Zn}_2(\text{bpdc})_2(\text{bpee})$ (bpdc = 4,4'- biphenyldicarboxylate; bpee = 1,2 – bipyridylethene) or also known as Rutgers' Porous Material 3 (RPM-3), will be used as a chemical sensor for the detection of olefins such as ethylene. A partially oriented RPM-3 thin film was solvothermally grown on a glass substrate using a method known as Pulsed Laser Deposition (PLD). This film will be utilized for the selective detection of 100 ppm $\text{C}_2\text{H}_4/\text{N}_2$ by post-functionalizing with AgNO_3 .



U11 New triosmium clusters with two bridging ligands

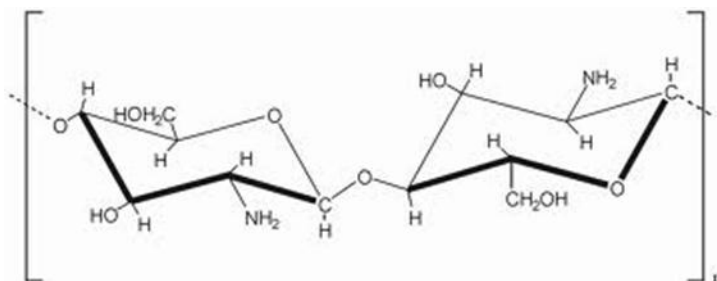
Nigel Gwini (nxg10a@acu.edu) and Gregory L. Powell. Department of Chemistry & Biochemistry, Abilene Christian University, Abilene, Texas 79699

Recent research has revealed anticancer properties of several osmium cluster complexes. A few of the cluster complexes in the studies contained two bridging ligands such as hydride and hydroxide. Other osmium clusters with two different bridging ligands are known and should be tested, but they are not easy to prepare in good yield. Since microwave heating has enabled the rapid preparation of metal complexes in our laboratory, we investigated the possibility of improving the conventional methods of preparing $\text{Os}_3(\mu\text{-X})(\mu\text{-Y})(\text{CO})_{10}$ clusters. Most reactions were carried out by reacting $\text{Os}_3(\text{CO})_{10}$ with another reagent (halogen, alcohol, etc.) in a microwave reactor. We also attempted to synthesize several new osmium clusters with two different bridging ligands such as bromide and methoxide.



U12 Electrospinning hollow chitosan fibers for enzyme immobilization

Eyerusalem Mamo (ehm090020@utdallas.edu) and Kenneth J. Balkus, Department of Chemistry and the Alan G. MacDiarmid Nanotech Institute, University of Texas at Dallas, Richardson TX 75080



Chemical structure of chitosan

Chitosan is a cationic polysaccharide, which is derived from an extra cellular matrix exoskeleton of autaceans. Its properties of immunogenocity, biodegradability, non-toxicity and wound healing properties make it to be favorable to be used in medical fields. Using a variety of inner core solutions along with concentric electrospinning, we are generating chitosan hollow fibers. The immobilization of enzymes within these hollow fibers makes them potential membrane reactors.



U13 Synthesis and characterization of zeolites and metal organic frameworks

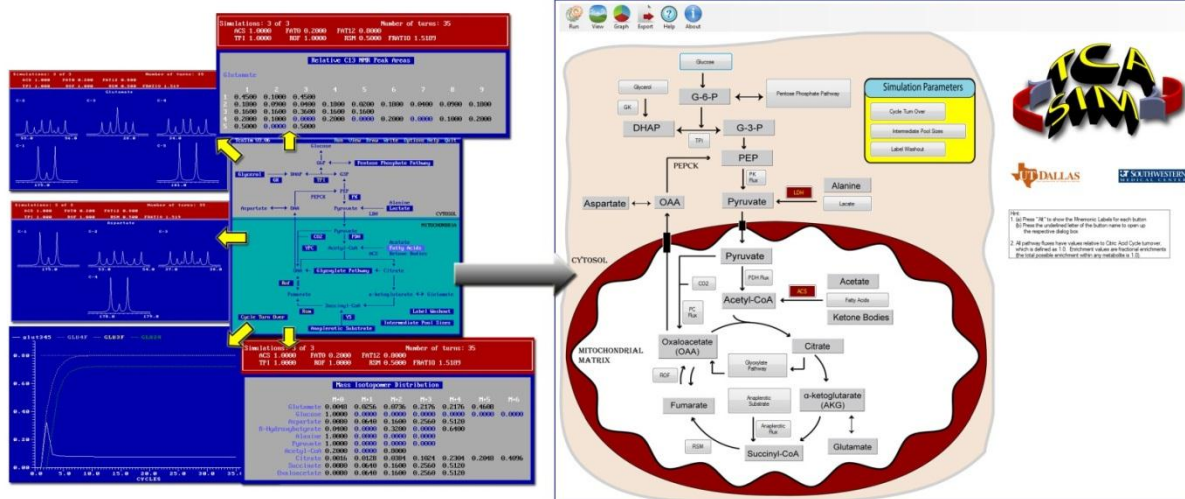
Anh Vu (anh.vu@utdallas.edu) and **Kenneth J. Balkus Jr.**, University of Texas at Dallas, Department of Chemistry and the Alan G. MacDiarmid Nanotech Institute, Richardson, TX 75080

There is growing interest in using natural zeolites and metal-organic frameworks (MOFs) as membrane materials for many applications, particularly catalysts and membrane separations. Synthesized zeolites, such as TNU-10, and MOFs, such as STU-1, have been shown to have microporous structures and interesting catalytic properties. The use of these materials as membranes would show unique separating opportunities. Pulsed laser deposition has been shown to be a precise method for fabricating thin films. STU-1 and TNU-10 were synthesized and characterized. Results for the synthesis of the zeolites and MOFs will be presented.



U 14 Translating the power of tcaSIM, a program that simulates isotopomer analysis-based intermediary metabolism, into a graphical interface

Sabin Kshattri¹, **Abhishek Chhetri**², **F. Mark H. Jeffrey**³, **A. Dean Sherry**^{1,3}, ¹Department of Chemistry, University of Texas at Dallas, Richardson, TX 75080, ²Department of Computer Engineering, University of Texas at Dallas, Richardson, TX 75080, ³Advanced Imaging Research Center, UT Southwestern Medical Center, Dallas, TX 75390



tcaSIM is a program that provides simulation of intermediary metabolism based on results of ¹³C tracer studies. The user can enumerate important parameter values, such

as relative flux through a certain pathway or the ¹³C enrichment level and pattern on a metabolite, and obtain simulated experimental data including ¹³C NMR spectra with peak and multiplet area information, ¹³C enrichment, and mass isotopomer distribution of several metabolites. It is also possible to generate multiple simulations to study the dynamics of metabolism, for example the evolution of different isotopomers with each turn of the citric acid (TCA) cycle. This program provides comprehensive information on the functioning of different metabolic pathways, but is limited in utility by its unintuitive, rather obsolete DOS-based framework, and its requirement of some level of prior knowledge of Character User Interface. Translating this program into a user-friendly Windows interface will make it very useful to a wide range of users from college students to a physician diagnosing metabolic disorders.



U15 Synthesis of biologically important novel pyridobenzimidazoles attached to indole or benzo[b]thiophene structures

Kimberly Mendoza (kmendoza@smu.edu) and **Edward R. Biehl**. Department of Chemistry, Southern Methodist University, Dallas, Texas 75275

The pyridobenzimidazoles *N*²-phenylpyridine-2,3-diamine were prepared from corresponding nitro compounds by tin chloride di-hydrate reduction and microwave irradiation under solvent free conditions. Furthermore, the starting nitro compounds were prepared from 2-chloro-3-nitropyridine and suitably substituted aniline under MW conditions. A new synthetic method was developed that provides ready access to a novel pyridobenzimidazoles derivatives. In addition, a synthetic route for the preparation of amines under solvent free conditions was demonstrated. Lastly, detailed biological activity studies (antibacterial, fungal, cancer and neuroprotective kinase inhibitor activity) of these important compounds are being carried out and preliminary results indicate that many of these compounds exhibit excellent neuroprotecting properties.



U16 Mechanism for the highly regioselective chlorination of anisole with household bleach

Michelle Baalman¹ (mbaalman@gmail.com), **Robert G. Landot**,² and **William H. Hendrickson**,¹ Department of Chemistry, University of Dallas, Irving, TX, 75062¹ and Department of Chemistry, Texas Wesleyan, Ft. Worth, TX, 76105²

The chlorination of anisole using commercial bleach provides a promising alternative to many current methods, which exhibit poor regioselectivity and use toxic and expensive materials. Knowing the mechanism of this reaction will help to optimize synthesis methods. Either an electrophilic aromatic substitution or a single electron transfer mechanism is possible. These mechanisms may be distinguished by measuring the relative reactivities of dimethoxy benzenes, and also by using a cyclopropyl probe to trap a radical intermediate. Our results show that the mechanism of anisole chlorination is electrophilic aromatic substitution.



U17 Selective hydrogenation of acetylene in ethylene over Au catalysts

James D. Wheeler, Jr.¹ (evangelist08@gmail.com), Xiaoliang Yan¹, Arjun R. Malipeddi¹, Ben W.L. Jang¹, and Lin Wen-Yuan², ¹ Texas A&M University- Commerce, Department of Chemistry, Commerce, TX 75428, ² Sid Richardson Carbon and Energy Co, Fort Worth, TX 76106

This study investigates the effectiveness of gold catalysts for selective hydrogenation of acetylene in the presence of large excess of ethylene. 5% & 1% gold catalysts were chosen for examination under varying parameters. One of the Au catalysts was prepared by deposition-precipitation method on TiO₂ support and the others were prepared by photocatalysis process. Before reaction, catalysts were reduced in hydrogen for 1 hour at 250°C or 400°C. The reactions were carried out at a space velocity of 60,000 cc/g/hr with 20:1, 10:1, 5:1, and 2:1 of hydrogen to acetylene molar ratios at temperatures from 50°C to 400°C.

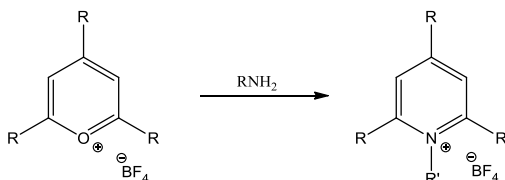
Among the catalysts tested, the 1% Au catalyst prepared by photocatalysis process produces the highest yield of ethylene, ~87% at a temperature of 250°C a 5:1 ratio of hydrogen to acetylene after being reduced for one hour at 250°C, and. The catalyst has been found to be stable for up to twelve hours under these conditions. Results and discussion on catalytic activity, such as conversion, selectivity and yield, and catalyst characterization, including Au loading, surface area, pore size distribution and coking, will be reported.



U18 Synthesis of pyridinium salts with possible biological activity

Holland Korbitz (holland_korbitz@baylor.edu), Nelson van der Velde, and Charles Garner, Baylor University, Waco, TX

Positively charged pyridinium salts provide a route for the possible improvement on the bioavailability of hydrophobic compounds and also an interesting interaction with different substrates. We are optimizing reaction conditions for making substituted pyrylium salts with primary amines to obtain pyridinium salts. Future work will be directed towards obtaining pyridinium salts from primary amines with known biological activity.



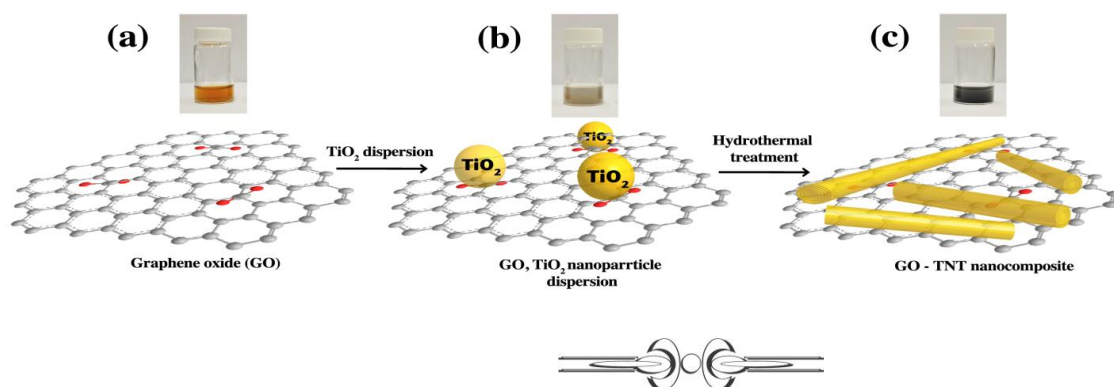
R = CH₃, Ph



U19 Reduced graphene oxide- TiO_2 nanotube composites for use as high-performance photocatalysts

Ruperto G Mariano¹, Sanjaya D Perera¹, Khiem Vu¹, Kenneth J Balkus Jr^{1,2}, Nijem Nour², Oliver Seitz², Yves Chabal^{1,2}, ¹University of Texas at Dallas, Department of Chemistry and the Alan G. MacDiarmid Nanotech Institute, Richardson, Texas, 75080; ²University of Texas at Dallas, Department of Materials Science and Engineering, Richardson, Texas, 75080

Titanium dioxide (TiO_2), while an excellent and widely investigated photocatalyst, has a wide band gap (3.2 eV.) Moreover, electron-hole recombination on TiO_2 limits the photocatalytic conversion of pollutants. It has been suggested that charge separation in TiO_2 nanoparticle-graphene composites is improved due to electrons moving onto the graphene. TiO_2 nanotubes (TNT) possess larger surface areas and shorter diffusion lengths compared to nanoparticles, and theoretically present superior synergistic effects with graphene. In this study TNTs were grown on graphene oxide for the first time. Additionally the synthesis of the TNTs also results in reduction of the graphene oxide to graphene. The TNT-graphene composites were characterized by XRD, Raman, SEM and TEM. The TNT-graphene composites were tested as catalysts for the photodegradation of organic dyes. The graphene-TNT nanocomposites exhibited improved photocatalytic efficiency in the degradation of malachite green.



Graduate Student Session A
Gorman A
Chair: Mr. John Lindsay

G01 Biophysical characterization of MiaE: an unusual non-heme diiron hydroxylase involved in tRNA post-transcriptional modification

Bishnu Subedi (bishnu.subedi@mavs.uta.edu) and Brad Pierce, Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Tx 76019

MiaE is a non-heme diiron enzyme which catalyzes the regioselective posttranscriptional allylic hydroxylation of 2-methylthio N-6 isopentenyl adenosine (A_{37}) of transfer RNA. By analogy to other members of the class II family of diiron enzymes, we hypothesize that specific protein-tRNA interactions are involved in gating delivery of electrons to the substrate-bound diiron cluster of MiaE. In principle, the modulation of the O_2 -reactivity at the active site is thought to be a function of protein-substrate interactions and thus will be an important additional area of investigation. In this work, we utilize Electron Paramagnetic Resonance (EPR) spectroscopy to monitor the binding of the anti-stem codon loop (ASL) of tRNA^{Phe} to the reduced *Salmonella typhimurium* MiaE recombinant enzyme. EPR microwave power saturation and temperature dependent experiments indicate that ASL-binding significantly alters the electronic relaxations rates of the diferrous MiaE active site but does not affect the Heisenberg exchange interactions ($H = JS_1 \cdot S_2$) between adjacent iron-atoms. This observation suggests that binding of ASL to MiaE induces a conformational change at the diiron site but does not alter the Fe-Fe distance. Additionally, the ASL-binding constant (K_D of $24 \pm 5 \mu M$) to the reduced MiaE enzyme was measured by EPR titration experiments.



G02 Development of small substrate surrogates for mechanistic and spectroscopic characterization of the O_2 -dependent tRNA modifying MiaE

Andra L. Carter, Frank W. Foss Jr., and Brad S. Pierce, Department of Chemistry and Biochemistry, University of Texas at Arlington Arlington, TX 76019

Post-translational modifications of transfer RNA (tRNA) are made to structurally diversify tRNA. These modifications are utilized to alter non-covalent interactions with the ribosomal machinery. Often, such modifications result in phenotypic changes related to cell metabolism, growth, and virulence. A variety of enzymes have been identified to be involved in post-transcriptional modification of tRNA. MiaE (2-methylthio-N-6-isopentenyl adenosine(37)-tRNA [$ms^{2i6}A_{37}$ -tRNA] monooxygenase) is one such enzyme. MiaE is a non-heme diiron enzyme isolated from *Salmonella typhimurium*, which catalyzes the O_2 -dependent hydroxylation of $ms^{2i6}A_{37}$ -bearing tRNA molecules that translate codons beginning with uridine. Three nucleoside substrate surrogates ($ms^{2i6}-A$, $H^{2i6}-A$, and $Cl^{2i6}-A$), and their corresponding hydroxylated products ($ms^{2io6}-A$, $H^{2io6}-A$, and $Cl^{2io6}-A$) were synthesized. In lieu of the native electron-transport chain, the non-heme iron peroxide shunt pathway was used to perform steady-state kinetic assays with MiaE. Results obtained from these assays show that MiaE can selectively hydroxylate small molecule surrogates of $ms^{2i6}A_{37}$ -tRNA, and provide insight into enzymatic substrate-specificity.



G03 Protein-protein interactions at the interface of human glutathione synthetase

M. De Jesus¹, **B. Ingle**², **T.R. Cundari**², and **M.E. Anderson**¹, *Chem & Biochem Dept, Texas Woman's University, Denton, TX 76204*¹; *Dept. Chem., CASCAM, University of North Texas, Denton, TX 76203*²

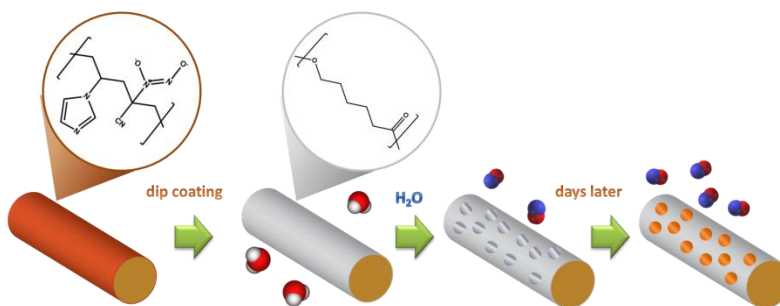
Human glutathione synthetase (hGS) synthesizes the important antioxidant glutathione. hGS is a useful model to study protein-protein interactions, because it is homodimeric and negatively cooperative toward its γ -glutamyl substrate (γ GC) [$h = 0.70$]. Thus, when the first γ GC binds, the affinity of the second γ GC for the second subunit of hGS decreases, down-regulating hGS activity and therefore intracellular GSH levels. It is likely that the negative cooperativity between the subunits travels through the interface. Computational analysis shows that amino acid residues S42, R221, and D24 are important to the dimer interface of hGS. Using site-directed mutagenesis, we changed the interface residues to alanine and then analyzed effects on hGS activity, stability, and cooperativity. Our results show that these hGS mutant residues remain negatively cooperative but have a 20-40% drop in activity and a 17- 35% drop in stability. Supported in part by NIH R15GM086833 (MEA), CASCAM (TRC), TWU REP grant (MEA) and Willis Clark scholarship (MD)



G04 Acrylonitrile-based fibers for enhanced wound healing with nitric oxide

Alysia Lowe (aal10000@utdallas.edu) and **Kenneth J. Balkus Jr.**, *The University of Texas at Dallas, Department of Chemistry, Richardson, TX 75080*

Nitric oxide (NO) is naturally synthesized by nitric oxide synthase, and plays an important role in physiological functions in the body. NO has been discovered as the endothelium-derived relaxing factor, allowing for vasodilation to occur in blood vessels, thus preventing platelet aggregation. NO has been shown to enhance wound healing. In this work, an acrylonitrile-co-1-vinylimidazole (AN/VIM) copolymer is electrospun and melt-spun to make materials for enhanced wound healing. The melt-spun material functions as a surgical suture type material, that demonstrates high durability and tensile strength, and the electrospun material functions as a bandage. Both can store and release NO. The NO molecular donor group, a diazeniumdiolate or NONOate, to form onto the AN comonomers. Each NONOate releases two molar equivalents of NO upon reaction with a proton source. Mechanical properties are maintained after the polymer is reacted with NO. To delay the release of NO from the suture, it is dipped in a solution of polycaprolactone (PCL) in toluene, creating a coating on the fiber. The biodegradable coating significantly slows release of NO compared to the uncoated fiber. This presentation will report on the NO release from these materials.



G05 Silver-functionalized $[\text{Zn}_2(\text{bpdc})_2(\text{bpee})]$ films: a luminescent metal organic framework for the detection of ethylene

Anne Marti (*amm094220@utdallas.edu*) and **Kenneth J. Balkus Jr.**, *The University of Texas at Dallas, Richardson, TX*

Thin films of the highly flexible, luminescent, three dimensional metal organic framework (MOF), $[\text{Zn}_2(\text{bpdc})_2(\text{bpee})]$ □ 2DMF (bpdc = 4,4'-biphenyldicarboxylate; bpee = 1,2-bipyridylethylene) were prepared by pulsed laser deposition (PLD) followed by a solvothermal treatment. The MOF film was then functionalized with $\text{Ag}_2(\text{NO}_3)_2$ that binds to the bpee linkers. The Ag functionalized MOF in its activated form exhibits improved N_2 and Ar uptake indicating the framework is more open. The reversible binding of ethylene by the Ag functionalized MOF was monitored by Fluorescence and Raman spectroscopy. These findings hold promise for this MOF to be used as a chemical sensor for olefins.



G06 Fabrication and characterization of novel metal organic framework stabilized immiscible polymer blend membranes for gas separation

Nimanka Pathum Panapitiya (*npp081000@utdallas.edu*) and **John P. Ferraris**, *University of Texas at Dallas, Richardson, TX*

Polymer blends offer a great potential to combine the high gas permeability of one polymer with the high gas selectivity of another but often comprise incompatible materials leading to uncontrollable phase separation. Immiscible polymer blends have been compatibilized with nanoparticles to obtain advanced materials for various applications, especially those needing a high surface area, but not have been extensively explored for the fabrication of gas separation membranes. We report a new class of mixed matrix membranes for gas separations in which two immiscible polymers with micro-scale domains are compatibilized with metal organic frameworks (MOFs). An advantage of this approach is the simultaneous contribution of MOFs both as a polymer compatibilizer as well as a molecular sieve for improved gas separation. The fabrication, characterization and permeability data of the polymer blend MMMs is presented.



G07 Spin-coated mixed-matrix membrane for gas separation at high pressure and high temperature

Jing Liu (jxl091120@utdallas.edu), Grace Jones D. Kalaw, Kenneth J. Balkus, Jr., John P. Ferraris, Inga H. Musselman, Department of Chemistry, The University of Texas at Dallas, Richardson, TX 75080

Membranes for H₂/CO₂ separation produced in a water gas shift reactor need to be stable at 300 °C and 30 atm. Mixed-matrix membranes (MMMs) were prepared from zeolitic imidazolate framework-8 (ZIF-8) and polybenzimidazole (PBI). ZIF-8 has a pore aperture of 0.34 nm, and is stable under hydrothermal conditions. PBI has a high T_g (418 °C), a H₂ permeability of 2.59 Barrers, and a H₂/CO₂ selectivity of 24. Compared to PBI, a 35% (w/w) ZIF-8/PBI MMM exhibits an increased hydrogen permeability of 5.36 Barrers and a somewhat lower H₂/CO₂ selectivity of 16. To improve H₂/CO₂ selectivity, a thin PBI layer was spin-coated onto the surface of the MMM. Scanning electron microscopy showed that the PBI layer was dense and uniform and that the PBI layer-MMM interface was absent of voids. The permeability and selectivity properties were tested at 35 °C and 3 atm, and high pressure, high temperature measurements are ongoing.



G08 Formation of gold nanoparticles *in situ* while electrospinning a polymer/Au⁺ solution under uv light

Fadwa Anka (fha041000@utdallas.edu) and Kenneth J. Balkus, Jr., University of Texas at Dallas, Richardson, TX

Gold nanoparticles (AuNP) were formed, in situ, while electrospinning a polyacrylonitrile (PAN) solution of HAuCl₄ under UV-light without using heat or chemical reducing agents. The resulting fibers were 200 to 400 nm as SEM images revealed, and their color was purple due to the formation of Au nanoparticles inside and on the surface of the nanofibers. TEM images showed spherical and uniformly dispersed particles inside the polymer nanofibers. The concentration of Au⁺ in the PAN solution is directly proportional to the size of the generated particles, with average diameter of 2.4 nm and 5.8 nm for the 0.044 M and 0.022M solutions, respectively.



G09 Carbon nanofibers from electrospun PAN/6FDA-NDA as electrodes for electrochemical double-layer capacitors

Jeliza S. Bonso (jsb082000@utdallas.edu) and **John P. Ferraris**, Department of Chemistry and the Alan G. MacDiarmid Nanotech Institute, University of Texas at Dallas, Richardson, TX 75080

Enhancement of performance of electrochemical double layer capacitors (EDLCs) can be achieved by using carbon materials with high electrical conductivity and high surface area as electrodes and an electrolyte with a high working voltage. In this study, we fabricated freestanding carbon nanofiber mats through electrospinning of precursor polymers. In this way, the use of binders, which not only add unwanted weight to the device but also block the electrolyte's access to pores in the electrodes, can be eliminated. We used polyacrylonitrile, which is a known precursor for carbon fibers, and 6FDA-NDA, a polyimide with a known high fractional free volume. The carbonized electrospun fiber mats were fabricated into coin-cell type (CR2032) capacitors and tested using cyclic voltammetry and galvanostatic charge-discharge tests in EMITFSI electrolyte which has a working voltage of ~4 V. Improvements in specific capacitances were observed as the amount of 6FDA-NDA wrt PAN was increased. From a 20% 6FDA-NDA (wrt PAN), the carbon nanofiber electrodes gave a specific capacitance of 105 F/g. Energy and power densities were also calculated to be 56 Wh/kg and 1.7 W/kg, respectively, at a discharge current density of 1 A/g.



G10 Asymmetric mixed matrix membranes fabricated using a spin coating technique

Sumudu Wijenayake (snw081000@utdallas.edu) and **John P. Ferraris**, University of Texas at Dallas, Richardson, TX

6FDA based polyimides offer thermal stability and remain as flexible membranes even upon incorporation of a high loading of additives. Mixed matrix membranes (MMMs) were fabricated incorporating zeolitic imidazolate framework-8 (ZIF-8) in 6FDA-durene up to 100% (w/w) loading, and a large (765%) increase in H₂ permeability was observed without a loss in H₂/CO₂ selectivity. A thin layer of the polymer was spin coated on to the MMMs followed by surface cross-linking of the skin using ethylene diamine (EDA), which led to a greatly enhanced H₂/CO₂ gas selectivity of 28. The permeability selectivity data are promising for hydrogen separation and lie above the Robeson upper bound for H₂/CO₂ separation. The membranes were characterized using ATR-IR, TGA, X-ray diffraction and SEM. The fabrication and characterization of the membranes along with the permeability and selectivity data will be presented.



G11 Electrospun core-shell Nafion/enzyme membranes for biofuel production

Daniel Tran (dnt019000@utdallas.edu) and **Kenneth J. Balkus Jr.**,

University of Texas at Dallas, Department of Chemistry and the Alan G. MacDiarmid Nanotech Institute, Richardson, TX 75080

In a previous study, cellulase fibers were successfully fabricated through core-shell electrospinning. In our study, we have electrospun b-glucosidase and cellulase fibers with a Nafion outer shell. Fibers provide a higher surface area when compared to protein immobilized on films, translating to higher active site accessibility and activity. The outer shell Nafion helps to hydrolyze cellulose which then is broken down to glucose by enzymes in the inner core. These fibers can potentially be incorporated as reactive membranes for the production of biofuels.



G12 Utilization of continuum models for nanosolids in soft matter environments

R. J. K. Udayana Ranatunga (uxr072000@utdallas.edu) and **Steven O. Nielsen**, *Department of Chemistry, University of Texas at Dallas, Texas 75080*

The steady improvement of computing power has fueled recent advances in computational modeling techniques. Among these techniques, the molecular dynamics simulation method is important because of its capability to probe physical processes in complex systems with extremely high spatial and temporal resolution. Systems containing nanoscaled solids in soft matter environments, such as aqueous dispersions of carbon nanotubes or C₆₀ fullerenes in cell membranes, are examples of systems where such resolution is required and experimental characterization is difficult. Here, through MD simulation results, we highlight advantages in using simple continuum models to represent nanosolids in soft matter. The use of such models allows us to test theories, investigate the effect of particle size on system behavior, and measure quantities such as solvation free energy and dimerization free energy. The use of such tools offers insight into these complex systems and better equips investigators to design and control their behavior.



G13 Reduced computational costs in the correlation consistent Composite Approach (ccCA) through explicitly correlated methods

Andrew Mahler (andrewmahler@my.unt.edu) and **Angela K. Wilson**, *University of North Texas, Denton, TX*

The prediction of energetic properties within “chemical accuracy” (1 kcal/mol) from well-established experiment is a major conundrum in computational chemistry due to the computational cost in terms of computer time, memory, and disk space needed to achieve this level of accuracy. Our group has developed a new type of *ab initio* model (or composite) chemistry, the correlation consistent Composite Approach (ccCA), which enables such accuracy to be possible, on average, but at reduced computational cost. Composite methods combine a series of less accurate quantum mechanical approaches to mimic the energetic prediction that would be possible with a much more accurate, though much more costly approaches. We have further reduced computational costs using a number of different strategies. In this work, we have utilized explicitly correlated methods within ccCA to accomplish this reduction. We discuss the strategy used, the cost savings achieved, and the accuracies possible using this method.



G14 Determination of equilibrium geometries using ccCA energy gradients

Matthew J. Carlson (*mjc0251@unt.edu*), Wanyi Jiang, Angela K. Wilson, Center for Advanced Scientific Computing and Modeling (CASCaM), Department of Chemistry, University of North Texas, Denton, TX 76203-5070

The correlation consistent Composite Approach (ccCA) has been shown to predict energetic data such as enthalpies of formation, ionization energies, and electron affinities within 1 kcal/mol, on average, from experiment for main group species, and at a reduced computational cost as compared to CCSD(T) with a large basis set. We have investigated the use of ccCA energy gradients to optimize equilibrium geometries of a set of closed-shell molecules. Within ccCA, several different schemes have been considered for extrapolation of properties (energies, and now gradients) to the complete basis set (CBS) limit. Of these schemes, the Peterson extrapolation has been determined to provide equilibrium geometries that most closely match experimental data. In order to reduce computation time, the scalar relativistic correction was not included in the gradient extrapolation, with an insignificant effect on the quality of results. The structures determined using the ccCA gradient-based optimization are in close agreement with experimental data, with a mean absolute deviation (MAD) of 0.10 picometers for bond lengths and 0.2 degrees for bond angles for the set of molecules considered.



G15 Development of a solvated composite method: The Solvated correlation consistent Composite Approach (Solv-ccCA)

Amanda G. Riojas and Angela K. Wilson, Department of Chemistry and Center for Advanced Scientific Computing and Modeling (CASCaM), University of North Texas, Denton, Texas 76203-5070

A solvated composite approach has been developed, incorporating the extensively parameterized SMD universal solvation model of Cramer and Truhlar into the correlation consistent Composite Approach (ccCA). This new Solv-ccCA methodology extends the ccCA family to the accurate prediction of theoretical pK_a s to within 2 pK_a units of experimental values. These calculations utilize a thermodynamic cycle which combines gas-phase and solution-phase calculations. Approaches which do not include a thermodynamic cycle for pK_a calculations have also been previously developed but often rely on the experimental values of reference acid molecules. Thermodynamic cycles can be considered to be more independent of experimental values and more appropriate for the pK_a calculations employed in the Solv-ccCA method. Several density functionals were also evaluated for use with SMD and for comparison to Solv-ccCA. The mean absolute deviation (MAD) from experiment for Solv-ccCA on a set of twenty substituted pyridines is 1.58 pK_a units. On average, Solv-ccCA exhibits higher accuracy when compared to the performance of the density functionals examined.



G16 The effect of carboxylic acid functionality on single-walled carbon nanotube cytotoxicity

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The cytotoxicity of carboxylated single-walled carbon nanotubes (SWNTs) is ambiguous in the literature. The process of functionalizing SWNTs with carboxylic acids generates amorphous carbon species, which increases the potential sources of toxicity. As-received SWNTs were carboxylated using nitric acid reflux for 2 to 16 h. Raman spectroscopy and atomic force microscopy were used to investigate chemical and physical changes, respectively. SWNT defects increased and SWNT lengths decreased with increasing reflux time. X-ray photoelectron spectroscopy was used to measure percent carboxylation, which increased up to 8 h and then decreased. SWNT cytotoxicity on NRK cells increased with increasing reflux time, but not with increasing percent carboxylation. The results of this study indicated that amorphous carbon species generated during the carboxylation process were the most probable source of cytotoxicity.



G17 Surfactant peptide/single-walled carbon nanotube (SWCNT) composites with altered electronic properties

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Charge transfer between electron-donating molecules and SWCNTs alters SWCNT electronic properties and thereby increases their applicability in carbon-based nanoelectronics. The current study investigates the interaction of SWCNTs with a series of aromatic moieties bearing electron-donating substituents including amine, dimethylamine, and hydroxyl groups, as well as nitrogen-containing heterocycles such as indole and pyridine. The aromatic functional groups, which interact with the SWCNT surface via π -stacking, were incorporated into the *N*-termini of short amphiphilic surfactant peptides. The amphiphilicity of the peptides helped to generate stable aqueous SWCNT dispersions. The electronic properties of the resultant composites were analyzed using Raman and scanning tunneling spectroscopy (STS). The downshift of the Raman G-band of all composites with respect to a reference SWCNT composite, prepared with a peptide containing an unsubstituted phenyl ring, indicates charge transfer from the peptide to the SWCNT surface (i.e., *n*-type doping). STS dI/dV spectra of the composites further confirmed the *n*-type doping of the SWCNTs by these peptides.



G18 A molecular dynamics investigation of single walled carbon nanotube dispersion by surfactant peptides

Blake Wilson (bxw109120@utdallas.edu) and **Steven Nielsen**, *University of Texas at Dallas, Richardson, TX*

Single walled carbon nanotubes (SWNTs) are intrinsically hydrophobic and tend to form insoluble bundles in aqueous solution. Separation of these bundles and solvation of the SWNTs thus requires the use of dispersing agents. Surfactant peptides (SPs) are short peptide chains that contain on one end a hydrophobic group and on the other a hydrophilic group. It has been experimentally observed that SPs act as a dispersing agent for SWNTs and that changing the hydrophobic terminus affects the efficiency of the dispersion. The underlying dynamics of this process cannot be observed experimentally. Here we use Molecular Dynamics (MD) simulations to explore the dynamics of SP assembly on a SWNT and the thermodynamics of SP-dispersion of SWNTs. The results of this study provide insight into the experimental results of SP dispersion of SWNTs, and the effect of varying the terminal moiety on dispersion efficiency.



Graduate Student Session B
Gorman B
Chair : Dr. Moji Bonakdar

G19 A titanium potential using the multi-state modified embedded atom method

Josh Gibson (*liquid.ice.007@gmail.com*) and **Angela K. Wilson**, *University of North Texas, Denton, TX*

A titanium potential has been constructed using the Multi-State Modified Embedded Atom Method (MS-MEAM)¹ formalism. Using first-principles calculations on selected crystalline reference structures of varying symmetries, the MEAM embedding functions, pair potential, and angular screening functions were determined. Calculations using MS-MEAM show that it is successfully capable of reproducing energies for a range of crystalline symmetries. Also, transformation pathways between reference structures have also been constructed using MS-MEAM and compare very well with first-principles calculations. Further implementation of MS-MEAM will focus on comparison to experiment and other embedded atom methods.

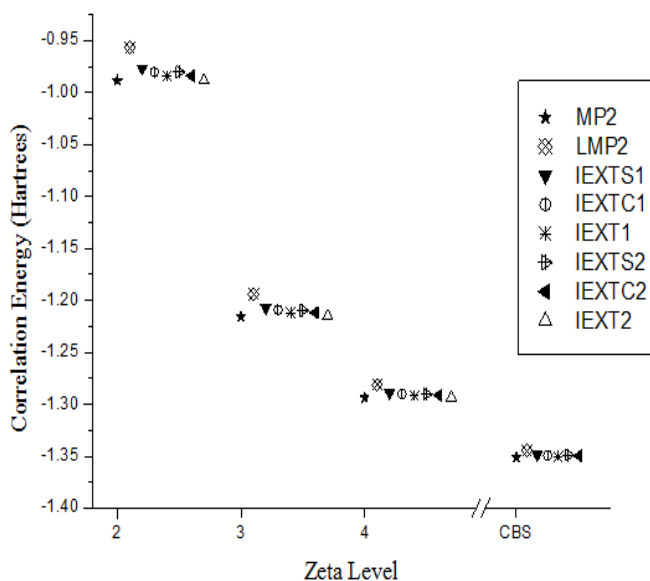
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G20 Recovery of correlation energy via local ab initio methods

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Achieving accurate properties for large compounds (over ~20 non-hydrogen atoms) is a challenge in computational modeling due to the computational scaling of ab initio methods. Therefore, reducing the computational resources necessary for these calculations has been a research interest for theoretical chemists. Local orbital approaches have been investigated with the goal of maintaining accuracy while reducing computational cost (i.e., RAM, Disk, CPU time). The performance of local Møller-Plesset second-order perturbation theory (LMP2) is investigated for a series of correlation consistent basis sets including cc-pVDZ, cc-pVTZ, and cc-pVQZ. The correlation energies were extrapolated to the complete basis set (CBS) limits using various schemes for comparison. Local method domain extensions, including strong, close and weak pairs are assessed in comparison to non-local MP2. The impact of extrapolation method and domain choice upon the correlation energy for each level of basis set is presented.



G21 Utility of MR-ccCA in reproducing potential energy curves and constants of diatomic molecules containing third-row elements

Christopher South and **Angela Wilson**, *University of North Texas, Department of Chemistry and Center for Advanced Scientific Computing and Modeling (CASCAM), Denton, Texas*

The potential energy curves for diatomic molecules containing third-row elements were examined using the multireference correlation consistent composite approach (MR-ccCA) to determine the applicability of the new approach for these systems. MR-ccCA is an *ab initio* composite method which is designed to replicate energies that, in principle, would be obtained using “MRCC”(fc1,dk)/aug-cc-pCV ∞ Z-DK, but instead uses a series of less accurate, albeit, less computationally costly (in terms of computer time, memory, and disk space). In earlier work, MR-ccCA was proven to be effective in reproducing potential energy curves for lighter molecules such as O₂, N₂, and C₂¹. As the methodology was not designed, per se, for potential energy curves, particularly due to the additive nature of the methodology, it was surprising to observe the remarkably smooth potential energy curves that resulted. To consider this phenomenon further and to consider the utilization of MR-ccCA across more of the periodic table, diatomic species including third-row atoms are considered herein. A number of properties have been considered including the dissociation energy D₀, well depth D_e, equilibrium bond length r_e, vibrational constants ((ω_e , $\omega_e x_e$) and rotational constants (B_e, α_e) and these properties have been compared with the experimental values. [1]Jiang, W.; Wilson, A. K. Multireference Composite Approaches for the Accurate Study of Ground and Excited Electronic States: C₂, N₂, and O₂. *J. Chem. Phys.*, **2011**, 134, 034101-1 – 034101-13



G22 Breaking the slow water exchange barrier in the design of functional PARACEST agents for MRI

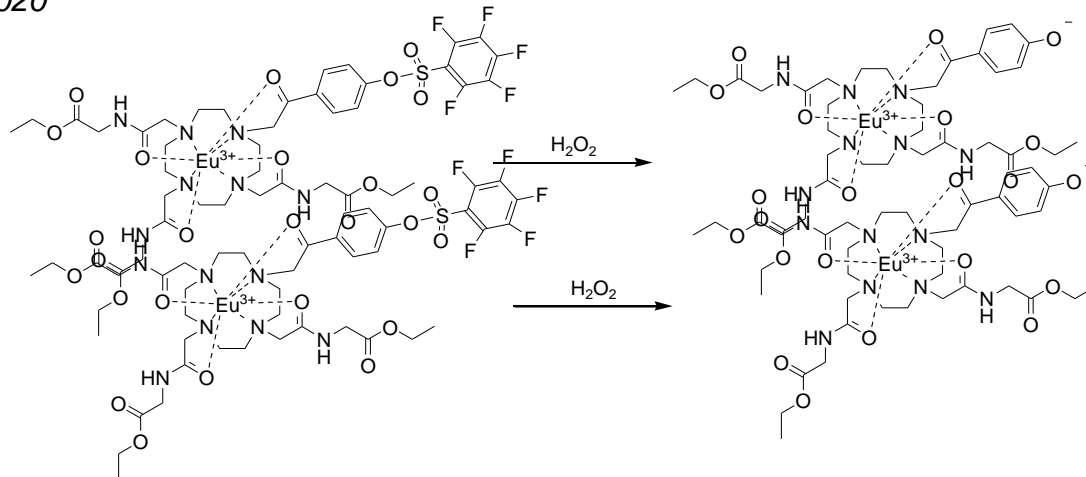
W. Shirangi K. Fernando (wkf090020@utdallas.edu) and **A. Dean Sherry**,
Department of Chemistry, University of Texas at Dallas, Richardson, TX

Magnetic resonance imaging (MRI) contrast agents have become an important tool in clinical medicine today. Current clinically used contrast agents work by shortening the longitudinal (T₁) and/or transverse (T₂) relaxation times of the protons in their close proximity. Although widely used, these agents have limited physical properties for further development as MRI contrast agents that will provide functional and anatomical information. Paramagnetic chemical exchange saturation transfer (PARACEST) agents have emerged to overcome these limitations. Image contrast is obtained using slower water exchange properties of the contrast agent that contain water molecules exchanging with bulk water. Eu(III)-DOTA-tetraamide complexes are the most widely studied group of PARACEST agents. Previous studies have shown that charge, polarity and bulkiness of the side chains could alter the bound water lifetimes of these complexes. Carboxylate groups, small hydrophobic groups and diethyl-phosphonate groups all tend to slow the water exchange rate. The current project focuses on building a small library of DOTA-tetraamide PARACEST agents with chemical features with more favorable water exchange kinetics than already reported.



G23 A New PARACEST agent for the detection and imaging of hydrogen peroxide

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A europium(III) DO3A-tris(amide) based complex was developed for the detection of hydrogen peroxide. The pentafluorobenzenesulfonyl unit of the probe reacts with hydrogen peroxide resulting in a 9 ppm downfield shift in the water exchange CEST peak and an increase in CEST effect. Ratiometric analysis at two different CEST frequencies showed a linear dependence on the concentration of peroxide demonstrating the potential of utilizing this agent in the detection and quantification of H_2O_2 *in vivo* by MRI.



G24 Density Functional Theory (DFT) for transition metal thermochemistry

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Transition metals have wide applicability from their use in catalysis such as hydrocarbon functionalization to their use in medicine such as soluble complexes to treat lymphomas. From diatomics to clusters to organometallics, transition metals are exploited for their unique properties such as conductivity and magnetic properties and industrial technologies including hydrogen fuel storage. To study small (less than fifteen non-hydrogen atoms) transition metal-containing molecules, high-level *ab initio* calculations are preferred for their accuracy. As the size of the molecule increases, density functional theory (DFT) is often employed. The design of exchange and correlation functionals for DFT is an active field of research. Since most density functionals are parameterized for main group molecules, the performance of a variety of density functionals has been examined for transition metal thermochemistry. With these results, the explicit design of a density functional for transition metals will be explored.

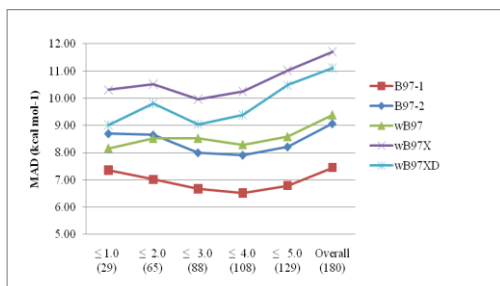


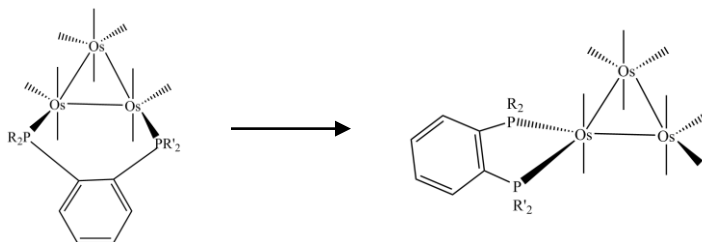
Figure 1. Performance of the B97 family of functionals for first row transition metal thermochemistry. (MAD is in comparison to experimental values)



G25 Rearrangement of diphosphine ligands in triosmium clusters: A computational study

Rebecca Weber (rebeccaweber@my.unt.edu), Angela Wilson and Michael Richmond, University of North Texas, Denton, TX

It has been reported¹ that the triosmium cluster $1,2\text{-Os}_3(\text{CO})_{10}(\text{P-P})$ isomerizes from the initial bridged structure to the chelated structure, $1,1\text{-Os}_3(\text{CO})_{10}(\text{P-P})$, shown below.



There are two proposed mechanisms for this movement¹. The first is termed a “merry-go-round” exchange, a one-step mechanism in which the CO ligands and the phosphine link all migrate about the equatorial plane of the cluster at the same time. The second is based on a conrotatory motion of the Os(2)-P bond, which then leads to a pairwise exchange of CO ligands and the phosphine across the Os-Os bonds.

The current study uses density functional theory to investigate the effects that different phosphine ligands have on the migratory preference.

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G26 Computational studies of CO₂ activation using transition metal catalysts

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CO₂ activation and conversion mediated by transition metal(TM) catalysts has been investigated. Homogeneous catalysis of the reverse water gas shift reaction $\text{CO}_2 + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{CO}$ was studied as a means to reduce CO₂. β -diketiminatometal models $\text{L}'\text{M}^{\text{I}}$ ($\text{L}' = \text{C}_3\text{N}_2\text{H}_5^-$; M = first-row TMs) were considered as potential catalysts. The thermodynamics of prototypical reaction pathways were simulated using B3LYP/aug-cc-pVTZ. Results show that middle series metal complexes result in more thermodynamically favorable properties; therefore, more detailed thermodynamic and kinetic studies were carried out for Mn, Fe, and Co complexes. Calculations show favorable thermodynamics and reasonable reaction barriers. On the other hand, heterogeneous catalysis of the reduction of CO₂ to CO were carried out on Fe, Co, Ni, and Cu fcc (100) surfaces, using the PBE density functional. Reaction energies were calculated using generalized gradient approximation (GGA), and reaction barriers were calculated using the climbing image nudged elastic band method. Calculations show spontaneous activation of CO₂, and favorable thermodynamics for the CO₂ decomposition, on Fe, Co, and Ni surfaces. In summary, an interesting energetic trend was found for both homo- and heterogeneous catalysis, as a function of metal: earlier metals tend to have stronger interaction with CO₂ than the later metals.



G27 Interactions of copper(I)-ethylene complexes supported by 1,3,5-triazapentadienyl ligands containing nitro group

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The purpose of this study is to understand the chemical interactions of copper metal with ethylene gas. New chelators containing nitro groups on 1,3,5-triazapentadienyl ligands were specially designed in this laboratory, and reacted with copper salts and ethylene gas. The net reactions resulted in copper(I) ethylene compounds, which are stable at room temperature for long periods of time. This observed phenomenon is unusual when compared to instability of copper salts with ethylene gas containing no chelators. Chemical bonding interactions between copper metal and ethylene of the synthesized complexes were investigated. It was found that the chelates are bonded to copper metal in U-shaped fashion. This work provides the valuable information of new copper(I) chelates binding to ethylene gas, and may lead to the development of new catalysts.



G28 Synthesis and characterization of multinuclear Ag(I) complexes possessing argentophilic interaction

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Metal catalyzed C-H activation via carbene insertion has drawn a considerable attention over the past few years to incorporate a variety of functionalities to alkanes in which readily available cheap materials are converted to more valuable products. Coinage metal complexes based catalysts with highly fluorinated ligands have shown much fascinating accomplishments in C-H activation. Hence a novel tunable bimetallic complex with a highly fluorinated metalloorganic ligand was designed for the C-H activation. In attempted syntheses an unexpected tetranuclear $\text{Ag}_4[3,5-(\text{CF}_3)_2\text{Pz}]_4[\text{Rbiim}]_2$ (Pz: pyrazolyl and Rbiim: 1,1'-R-2,2'-biimidazole; R : Me/ *n*-Pr) was obtained. The characterization of the complexes revealed that both the tetra nuclear silver(I) complexes consist of four pyrazole groups and two biimidazole groups as bridging ligand showing argentophilic interactions. Currently a modified approach is being followed by altering the substituent groups of the biimidazole ligands for the synthesis of the targeted dimer.

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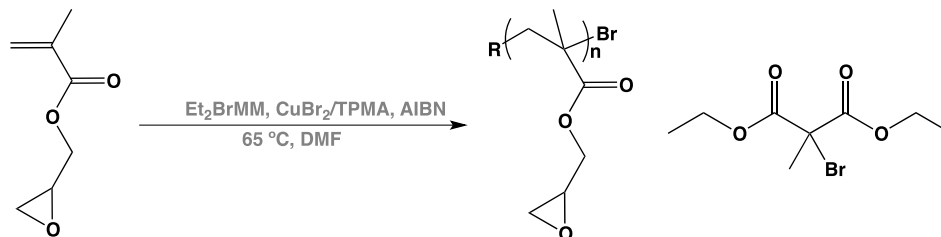
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G29 Synthesis of well-defined polymers with epoxide groups by atom transfer radical polymerization and their use as precursors of functional materials

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Atom transfer radical polymerization (ATRP) techniques that can be employed with a low concentration of Cu-based catalyst are of great interest in the production of well-defined functional materials as they can often reduce the need for extensive purification techniques, as seen in “classical” ATRP processes. One of these in particular, ICAR ATRP, has been successfully utilized to polymerize glycidyl methacrylate, an epoxide-containing monomer. Solvent and initiator studies were undertaken to optimize these conditions. The resulting epoxide-containing polymers were used as precursors of a number of different functional materials with potential applications in biological studies, education, industry, and more. The synthesis of biodegradable gels with applications in the field of NMR spectroscopy is also explored.



G30 Applications of exchange reactions at hypervalent iodine centers for the synthesis of polymeric materials

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(Diacyloxyiodo)arenes and I-acylbenziodoxoline-3-ones belong to the large group of org. hypervalent iodine (III) compds., which are able to exchange acyloxy ligands in various reaction media. The dynamic nature of the hypervalent I-O bonds as well as their easy homolytic cleavage under thermal and photochem. conditions allow for the synthesis of various polymeric materials under radical polymn. conditions, including hyperbranched macromols., polymer brushes and reversible gels. The efficiency of ligand ==exchange between the aforementioned compds. and polymerizable carboxylic acids, multicarboxylic acids, or other nucleophilic groups as well as synthetic applications (prepn. of polymeric materials with different architectures and degrees of functionalization) will be described.



G31 Synthesis of novel zeolitic imidazolate frameworks

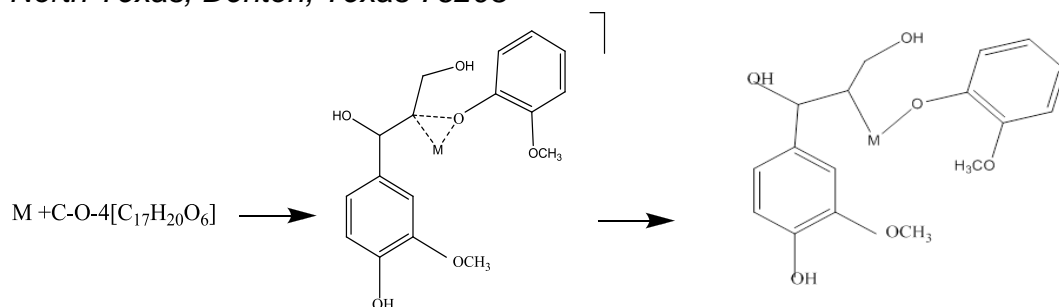
Sajani Basnayake (sab096120@utdallas.edu) and **Kenneth Balkus Jr.**, Department of Chemistry, University of Texas at Dallas, Richardson, Texas 75080

Zeolitic Imidazolate Frameworks (ZIFs), a family of Metal Organic Frameworks (MOFs), have large cavities with small pore apertures which makes them useful for separating small molecules. ZIF-8, $\text{Zn}(\text{2-methylimidazole})_2$ is one of the most promising representatives of ZIFs due to its very large pore size and high chemical and thermal stability. ZIF-7 which is constructed of Zn^{2+} ions bridged by benzimidazole linkers has exhibited H_2 separation capabilities. In this study, we report the formation of new crystalline phases that result from the hydrolysis of the solvent, DMF in the ZIF-8 synthesis; and in ZIF-7 synthesis, with the presence of aqueous KCl. X ray diffraction, Scanning electron microscopy (SEM) and IR spectroscopy were used to characterize the crystals.



G32 Transition Metal Catalyzed Oxidative Cleavage of $\text{C}_\beta\text{-O}$ Bond in $\beta\text{-O-4}$ Linkage of Lignin

Jiaqi Wang (wang.jiaqi@yahoo.com) and **Angela Wilson**, Department of Chemistry, University of North Texas, Denton, Texas 76203



Lignin is a potential alternative energy resource. However, lignin is still an underused biomass species because of its highly branched structure. To aid in better understanding this species, the oxidative cleavage of the $\text{C}_\beta\text{-O}$ bond in an archetypal arylglycerol $\beta\text{-aryl}$ ether ($\beta\text{-O-4}$ Linkage) model compound of lignin with Ni, Pt, Rh, CO and Fe species has been investigated. Reaction energies and activation energies have been studied to determine if these reactions are thermodynamically and kinetically feasible. Computational methods that have been applied include several density functional (B3LYP, B2PLYP, M06, M06L, B97D), CCSD(T) and the relativistic pseudopotential correlation consistent composite approach (rp-ccCA).



G33 Hydrothermal synthesis of Graphene-TiO₂ nanotube composites with enhanced photocatalytic activity

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In this study, TiO₂ nanotube (TNT)/reduced GO (hGO) composites were prepared by an alkaline hydrothermal process. This was achieved by decorating graphene oxide layers with commercially available TiO₂ nanoparticles (P90) followed by hydrothermal synthesis, which converts the TiO₂ nanoparticles to small diameter (~9 nm) TNTs on the hGO surface (Figure 1). The alkaline medium used to synthesize the TNTs simultaneously converts GO to deoxygenated graphene oxide (hGO). The graphene nature of hGO in the composites was confirmed by XRD, Raman, FTIR and XPS analysis. The photocatalytic performance of the hGO-TNT composites was evaluated for the photodegradation of malachite green. It was found that the composite with 10% hGO showed the highest photocatalytic activity, with a 3-fold enhancement in photocatalytic efficiency over pure TNTs. It is expected that the synthesis of “high surface area-small diameter” TiO₂ nanotubes and simultaneous conversion of GO to graphene like hGO “without using strong reducing agents” could be a promising strategy for preparing other types of carbon based TiO₂ nanotube composite photocatalysts.



G34 Au-CeO₂ Nanocomposites for photocatalytic applications

Anjalee D. Liyanage and **Kenneth J. Balkus Jr.**, *Department of Chemistry, The University of Texas at Dallas, Richardson, TX 75080*

CeO₂ nanorods functionalized with gold nanoclusters were prepared using photo irradiation. Thiolactic acid was used as the linker to control the size and the distribution of gold nanoclusters on CeO₂ nanorods. The products were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and UV-Vis spectroscopy. The photocatalytic activity of the nanocomposites were evaluated for photodecomposition of methylene blue. Preliminary results showed that the gold nanocluster decorated CeO₂ nanorods has a higher photodegradation rate compared to bare nanorods under the used experimental conditions.



G35 Selective hydrogenation of acetylene over Pd on ionic liquid loaded SiO₂ support

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Ionic liquid loaded supports (ILLS) for Pd as heterogeneous catalysts receive great attention for selective hydrogenation lately. This investigation focused on [Bmim][PF₆-] loaded silica supported Pd catalyst, using palladium acetylacetonate as the precursor. Selective hydrogenation of acetylene in a large excess of ethylene was used as a probe of selective hydrogenation reaction to test the capability of the catalyst. Reaction conditions used included reduction conditions of 100°C/2hr, 50°C/3hr and 25°C/3hr and H₂/C₂H₂ ratios of 2/1, 5/1, 10/1 and 20/1. The catalyst showed the highest catalytic activity with 10/1 ratio when reduced at 100°C/2hr. Reduction conditions of 100°C/2hr and 50°C/3hr had similar conversions and yields which were higher than that of 25°C/3hr with 10/1 ratio. Other catalysts on different supports, alumina and titania, were also tested in this study, silica generally leaded to higher catalytic activity by comparison. The catalyst also performed very good stabilities under 60°C/5hr, 90°C/5hr and 120°C/5hr reaction conditions with 10/1, 5/1, 2/1 ratios, respectively. The comparison of acetylene conversion, ethylene selectivity and ethylene yield of catalysts will be reported in details.



G36 Heterogeneous catalysis of Bio-diesel using starch based catalysts under experimental application of ultrasound

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This work offers an optimized method for producing bio-diesel using a starch based heterogeneous catalyst with the help of ultrasound technology. The research is based on the transesterification of oleic acid to methyl oleate which is deemed to be high grade bio-diesel. Catalyst were prepared with a wide variety of heating and sulfonation parameters both with and without ultrasound preparation. The transesterification reaction was carried out with heat and stirring and without heat under ultrasound. Our catalyst shows both high activity and stability and is able to be recharged if needed. The optimum conversion of oleic acid is achieved (99.8%) with a 140 mg of catalyst at room temperature using an ultrasound bath. Over the research period we have reduced effective reaction time from 6 hours to 30 minutes, and achieved maximum conversion this time period with 140 mg of catalyst. This new method demonstrates untested techniques in regards to bio-diesel and may help reduce the cost of commercially produced bio-diesel in the future.



Conjugated aromatic PPI: Characterization of structure, electronic spectra and thin films from soluble complexes

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The conjugated aromatic Schiff base polymers or poly (azomethines), such as PPI (poly(1,4-phenylenemethyldynenitrilo-1,4 -phenylenenitrilomethylidyne)), is thermally stable film and fiber forming materials that exhibit good mechanical strength. The detailed structure of this polymer has been studied because of its Schiff base (-CN=N-). The imine nitrogen on the backbone provides a Lewis base site which is reversible complexation and makes a thin and stable fiber. This polymer was prepared by solution polymerization of terephthalaldehyde, p-phenylenediamine and scandium triflate catalyzed in the methanol or NMP solution at room temperature. The yellow powders polymer was precipitated after 10h reaction. Its characterization was determined by FTIR spectra. The thin fiber was collected from electro spinning or core-shell electrospinning.

