60th Pentasectional Meeting of the American Chemical Society

Pittsburg, Kansas
April 10-11, 2015
Pittsburg State University Campus Map
909 East Ford St.
Pittsburg, KS 66762
60th Pentasectional Meeting of the American Chemical Society

Program and Abstracts
April 10–11, 2015
Pittsburg State University
Kansas Technology Center
909 East Ford St.
Pittsburg, KS 66762

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2015 Pentasectional Organization Committee
Charles J. Neef (Chair), Donna Zink, Khamis Siam, Ram Gupta, & Kris Mijares
Sponsors and Exhibitors
Meeting Sponsor

Polymer Chemistry Initiative

Creating the future...today!

College of Arts and Sciences
College of Technology
Kansas Polymer Research Center

Dr. Petar Dvornic
Department of Chemistry Chair and
Professor of Polymer Chemistry

Dr. Santimukul Santra
Assistant Professor of Polymer Chemistry

Dr. Ram Gupta
Assistant Professor of Polymer Chemistry

Dr. Jeanne Norton
Assistant Professor of Plastics Engineering Technology

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discover their traits through hands-on research
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of Chemistry, as well as in our renowned
Kansas Technology Center and Kansas Polymer Research Center.
The Kansas Polymer Research Center
is pleased to support the
2015 ACS Pentasectional Meeting

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Sponsors and Exhibitors

Analytical Chemistry Session Sponsor
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Shimadzu Instruments

Exhibitors
Oklahoma State University - Chemistry Department
Pittsburg State University - Polymer Chemistry Initiative
Pittsburg State University - Chemistry Department
Pittsburg State University - Graduate and Continuing Studies
Wyatt Technology Corp.
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:00-9:00 am</td>
<td>Registration (Main Entrance/Rotation)</td>
</tr>
<tr>
<td>8:30-9:30 am</td>
<td>Keynote Speaker (Auditorium Room S102)</td>
</tr>
<tr>
<td>9:30-10:30 am</td>
<td>Analytical Chemistry Room S103, Materials and Polymer Chemistry Room S110</td>
</tr>
<tr>
<td>10:30-10:50 am</td>
<td>Break (Main Entrance/Rotation)</td>
</tr>
<tr>
<td>10:50-11:50 am</td>
<td>Analytical Chemistry Room S103 (continued), Materials and Polymer Chemistry Room S111 (Session 1 continued), Materials and Polymer Chemistry Room S110 (Session 2 continued)</td>
</tr>
<tr>
<td>12:00-1:00 pm</td>
<td>Lunch/Oklahoma Chemist of the Year (Auditorium Room S103)</td>
</tr>
<tr>
<td>1:00-2:00 pm</td>
<td>Physical and Computational Chemistry Room S109, Organometallics Room S111, Inorganic Chemistry Room S110, Organic Chemistry Room S109, Nanoscience Room S120</td>
</tr>
<tr>
<td>2:00-3:00 pm</td>
<td>Poster Session (Lobby outside Room S103)</td>
</tr>
<tr>
<td>3:00-3:30 pm</td>
<td>Poster Awards and Closing Remarks (Auditorium Room S103)</td>
</tr>
<tr>
<td>3:30-4:00 pm</td>
<td>Pentasectional Planning Meeting (Conference Room S113)</td>
</tr>
</tbody>
</table>

Posters may be set up during any time prior to 9am
Poster Presenters, please be at your poster between 2:00pm-3:30pm (corridor outside Room S103) for the poster session.
The Oklahoma Chemist Award was initiated in 1971 and was primarily started by Dr. George R. Waller who was a faculty member in the Biochemistry Department at Oklahoma State University. Oklahoma is divided into five sections of the American Chemical Society, and each Section agreed to support this award on an annual basis. The concept for the award was to honor truly outstanding contributions made to the science and to the state by a chemist in recent years within the state of Oklahoma. Although originally designed to honor research chemists, an amendment was introduced in the 1980s to allow candidates to be nominated who had made extraordinary contributions to the area of chemical education whether it be to youth or to the public in general. Three such awards have been made to chemical educators over the years since the inception of the award in 1971. One award was to be given each year if a suitable candidate was identified from the research community or from education. The original award consisted of $500 and a handsome plaque formed in the shape of the state of Oklahoma.

One member from each of the five Sections was appointed to compose a reviewing committee to accept nominations which were to be received around February 1 of each new year. The date was to permit sufficient time for the winner to be selected and to receive the cash award and plaque at the next annual Pentasectional Meeting in the spring. The Pentasectional Meeting brings together chemists from academia and from industry within the state one time each year to present research results. It is the largest meeting of chemists in Oklahoma.

The OKLAHOMA CHEMIST AWARD is the most prestigious award given to a chemist within Oklahoma. The award now consists of $1000 as well as the plaque described above. A brief description of the accomplishments by the recipient are engraved on the plaque and are submitted, along with a photo of the winner, to Chemical and Engineering News for official publication in a forthcoming issue. Chemical and Engineering News is a major publication of the American Chemical Society and has world wide distribution.
Dr. A.K. Fazlur Rahman, professor of chemistry at the Oklahoma School of Science and Mathematics (OSSM), is the recipient of the 2015 Oklahoma Chemist Award. He has been an active and influential force in chemical education for the last two decades. Having coached many Chemistry Olympiad participants, he has established an impeccable record in national and international arenas. His students have earned gold, silver and bronze medals for the United States. Thus far, he has led 10 students at the US National Chemistry Olympiad camp (at the Air force Academy) and four in the International Chemistry Olympiad to carry the chemistry flag of Oklahoma. Additionally, he has promoted STEM education in Oklahoma by coaching TEAM+S (Test of Engineering Aptitude in Mathematics and Science) competition for the last 15 years. His students have consistently won state and national championships.

Dr. Rahman has initiated and developed the organometallic chemistry research program, the nation's first for a high school, while at OSSM. Currently, he has supervised more than 45 students with chemistry research mentorships. He has established a credential by securing instructional instrumentation and research support for high school students from various funding agencies. His contributions to a variety of chemistry outreach programs designed for K-12 students include: (1) empowering his junior and senior students to introduce chemistry principles to thousands of fourth and fifth graders, (2) providing chemistry workshops for middle school and high school teachers, and (3) serving as coordinator of E-team, which has visited numerous elementary schools to popularize science with chemical demonstrations. Dr. Rahman has been instrumental in developing ACS curricula in general chemistry and organic chemistry while in a high school setting. His students commonly receive chemistry course credit at state universities and other top institutions. Additionally, his students have attended chemistry programs at some of the most prestigious undergraduate and graduate schools in the nation. Many of his students are chemistry faculty members at Stanford, MIT, Georgia Tech and Johns Hopkins.

Dr. Fazlur Rahman earned B.Sc (Hons) in chemistry from Jahangirnagar University, M.A in organic chemistry from Brandeis University and Ph.D. in organometallic chemistry from The Australian National University. He is the recipient of the Stanford University Teacher Tribute Award for exceptional teaching (2003), the Sigma-Xi distinguish teaching award (2005), the American Chemical Society (ACS) South West Regional Award (2009), and the Research Opportunity Award from EpsCOR NSF in 2009. Dr. Rahman availed fellowship from the Ames Laboratory (1990-91), National Renewable Energy Laboratory (1995), Phillips Petroleum Company (1996-97), and the National Science Foundation (1998). He has held visiting positions at the University of Rochester (1995), Texas A&M (2012) and at the California Institute of Technology (2013). To his credit, Dr. Rahman has published more than 22 papers and has made more than 55 research presentations at national and international conferences. Apart from the Oklahoma School of Science and mathematics, Dr. Rahman has been teaching chemistry at the University of Oklahoma and the University of Central Oklahoma.
# 2015 Oklahoma Chemist Award History

## Past Recipients

<table>
<thead>
<tr>
<th>Year</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1971</td>
<td>Wayne White</td>
</tr>
<tr>
<td>1972</td>
<td>not awarded</td>
</tr>
<tr>
<td>1973</td>
<td>Otis C. Dermer</td>
</tr>
<tr>
<td>1974</td>
<td>Robert L. Banks</td>
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<tr>
<td>1975</td>
<td>Charles M. Starks</td>
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<tr>
<td>1976</td>
<td>Kang Yang</td>
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<tr>
<td>1977</td>
<td>Kenneth Darrell Berlin</td>
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<tr>
<td>1978</td>
<td>Gerard Kraus</td>
</tr>
<tr>
<td>1979</td>
<td>Lionel M. Raff</td>
</tr>
<tr>
<td>1980</td>
<td>Wayne F. Hower</td>
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<tr>
<td>1981</td>
<td>Alfred Clark</td>
</tr>
<tr>
<td>1982</td>
<td>Marvin M. Johnson</td>
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<tr>
<td>1983</td>
<td>Simon Wender</td>
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<tr>
<td>1984</td>
<td>E. J. Eisenbraun</td>
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<tr>
<td>1985</td>
<td>Dick van der Helm</td>
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<tr>
<td>1986</td>
<td>Sherril D. Christian</td>
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<tr>
<td>1987</td>
<td>Francis J. Schmitz</td>
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<tr>
<td>1988</td>
<td>Marvin K. Kemp</td>
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<tr>
<td>1989</td>
<td>Glenn Dryhurst</td>
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<tr>
<td>1990</td>
<td>Horatio A. Mottola</td>
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<td>1991</td>
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<tr>
<td>1992</td>
<td>Elizabeth Anne Nalley</td>
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<tr>
<td>1993</td>
<td>Bing M. Fung</td>
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<td>1994</td>
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<td>1995</td>
<td>Gilbert J. Mains</td>
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<tr>
<td>1996</td>
<td>Max P. McDaniel</td>
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<tr>
<td>1997</td>
<td>Donald L. Thompson</td>
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<td>1998</td>
<td>Roger E. Frech</td>
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<td>1999</td>
<td>Warren T. Ford</td>
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<tr>
<td>2000</td>
<td>Robert E. Howard</td>
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<tr>
<td>2001</td>
<td>George R. Waller</td>
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<td>2002</td>
<td>P. K. Das</td>
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<td>2003</td>
<td>James Weaver</td>
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<tr>
<td>2004</td>
<td>Daniel E. Resasco</td>
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<td>2005</td>
<td>Neil Purdie</td>
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<td>2006</td>
<td>Donald D. Knudsen</td>
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<td>2007</td>
<td>Ziad El Rassi</td>
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<td>2008</td>
<td>Joe Allison</td>
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<tr>
<td>2009</td>
<td>Richard A. Bunce</td>
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<tr>
<td>2010</td>
<td>Jiten Chatterji</td>
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<tr>
<td>2011</td>
<td>Dale Teeters</td>
</tr>
<tr>
<td>2012</td>
<td>Donna J. Nelson</td>
</tr>
<tr>
<td>2013</td>
<td>Tushar Choudhary</td>
</tr>
<tr>
<td>2014</td>
<td>Allen Apblett</td>
</tr>
<tr>
<td>2015</td>
<td>A.K. Fazlur Rahman</td>
</tr>
<tr>
<td>2016</td>
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Future Energy Needs

Conserve energy...do what you can...change to compact fluorescents which will save many billion watts of energy. The whole globe consumes, on average, 13 terawatts. Terawatts is the scale of energy. The unit of energy is “Joule” and this is the “Jewel” that we need to treasure, conserve, and handle with care. The presentation will provide a very simple physicist’s perspective on our future energy needs. An overview of fossil energy, fission energy, fusion energy, solar energy, hydrothermal energy, wind energy, and biomass energy will be given.

Biographical Sketch:

Dr. Pawan Kahol has been the Dean of Graduate and Continuing Studies, Dean of Research, and Professor of Physics at Pittsburg State University since 2012. After his Ph.D. in Physics from Panjab University in 1978, he has worked as a research associate/postdoctoral fellow at Leeds University (England) for 4 years, Stuttgart University (Germany) for over three years, and West Virginia University for two years. He worked at Wichita State University for 17 years and worked up through the ranks from Assistant Professor to Associate Professor to Professor to Chairperson and to Associate Dean of Graduate School. He then moved to Missouri State University as the Department Head of Physics, Astronomy, and Materials Science in 2005. He also served at Missouri State University as the Associate Dean of the College of Natural and Applied Sciences for two years and Interim Dean of Graduate College for one year.

Dr. Kahol has published nearly 180 refereed research papers including two review articles in physics, chemistry, and materials science. He has also made nearly 200 national/international/regional presentations. He has chaired many sessions at national/international meetings. He and his collaborators have received over 3 million dollars for research from external agencies.

Dr. Kahol is a recipient of the 2009 Carnegie Foundation for the Advancement of Teaching Missouri Professor of the Year award; 2010 Foundation Award for Teaching at Missouri State University, and 2003 Effective Teaching Award at Wichita State University. He has co-authored 16 volumes of solution manuals for both the calculus-based and the trigonometry-based introductory physics textbooks which have been published by Addison Wesley.
While the concept of sustainability has been around for a number of years, it has gotten much more attention in the food industry recently. One early definition, which came out of a 1987 UN conference, was that we be able to “meet present needs without compromising the ability of future generations to meet their needs”. There are several main areas in which the food industry can focus to be sustainable. One of the first is in agricultural practices. An example of one major effort is specifically for palm oil where companies have formed the Roundtable for Sustainable Palm Oil (RSPO). The organization has established standards to certify palm plantations as sustainable. Another area is packaging. This brings out one important consideration in that packaging is designed to protect the product and while one package may be bio-based or bio-degradable, it cannot compromise the quality of the product. Water is also a major consideration in agriculture and food processing. All of these as well as other factors influencing decisions on how the food industry can be sustainable will be addressed.

Biographical Sketch:

Sara Risch is the Director of Global R&D and QA for Popz Europe, a microwave popcorn company. Prior to joining Popz, she had her own consulting business, working with food, flavor and packaging companies. Sara moved away from consulting for a couple of years to serve as the Director of the School of Packaging at Michigan State University. She received her both her B.S. and Ph.D. in Food Science from the University of Minnesota. She has an M.S. in Food Science from the University of Georgia. Her work has focused primarily on microwave foods and food-package interactions. Dr. Risch was elected a Fellow of the American Chemical Society in 2012.
MoKanOk Section Governance

2015 Section Officers and Standing Committee Chairs

Donna Zink  Chair
Ram Gupta  Chair Elect
Jody Neef  Immediate Past Chair
Alexander Bednekoff  Secretary/Treasurer
Khamis Siam  Councilor, Nominations Committee Chair
Kris Mijares  Alternate Councilor
William Shirley  Newsletter/Publications Committee Chair
Dilip Paul  Chemistry Olympiad Committee Chair
Irene Zegar  National Chemistry Week Committee Chair
William Shirley  Webmaster

This 60th ACS Pentasectional meeting is being hosted by the MoKanOk local section of the American Chemical Society. For more information about our section, please visit our web site:

http://mokanok.sites.acs.org/
Schedule of Events

Friday
6:30 - 7:00 pm: Registration and Social

7:00 – 8:00 pm: Dr. Pawan Kahol (Auditorium S102)

Saturday
8:00-9:00 am:  Registration and Continental Breakfast
   On-Site Registration and Badge Pickup

8:30 – 9:30 am:  Keynote Speaker
   Dr. Sara Risch (Auditorium S102)

9:30-12:00 pm:  Technical Sessions
   Analytical Chemistry (S103)
   Materials and Polymer Chemistry-Session 1 (S111)
   Materials and Polymer Chemistry-Session 2 (S110)
   Organic and Biochemistry (S109)
   Environmental Chemistry (S120)
   Chemical Education (S120)

12:00-1:00 pm:  Lunch
   Oklahoma Chemist of the Year Award (Auditorium S102)
   Box Lunch

1:00-2:00 pm:  Technical Sessions
   Physical and Computational Chemistry (S109)
   Organometallic Chemistry (S111)
   Inorganic Chemistry (S110)
   Organic Chemistry (S109)
   Nanoscience (S120)

2:00-3:00 pm:  Poster Session

3:00-3:30 pm:  Poster Awards and Closing Remarks

3:30-4:30 pm:  Pentasectional Planning Meeting
### Technical Sessions Schedule

#### Analytical Chemistry (S103)

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Presenter(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:30-9:50</td>
<td>TA01</td>
<td>Enhancement of Catalytic Features of Heme Proteins Attached to Magnetic Nanoparticles</td>
<td>Gayan Premaratne, Oklahoma State University - Stillwater</td>
</tr>
<tr>
<td>9:50-10:10</td>
<td>TA02</td>
<td>pH Indicator to Enhance Surface Plasmon Resonance Imaging Detection of Weak Acids</td>
<td>Zainab Al Mubarak, Oklahoma State University, Stillwater</td>
</tr>
<tr>
<td>10:10-10:30</td>
<td>TA03</td>
<td>Morphologies controlled synthesis of CoS2 for enhanced electrochemical properties</td>
<td>E. Alqurashi, Pittsburg State University</td>
</tr>
<tr>
<td>10:50-11:10</td>
<td>TA04</td>
<td>Synthesis of Reduced Graphene Oxide and the Effects of Adsorption of Organic Compounds by Structure</td>
<td>Tye Chapman, University of Central Oklahoma, Oklahoma State University</td>
</tr>
<tr>
<td>11:10-11:30</td>
<td>TA05</td>
<td>Development of a Microfluidic Immunological Assay for the Detection and Identification of Bluetongue Virus and EHDV Induced Antibodies in Serum.</td>
<td>Mary Tappert, University of Central Oklahoma</td>
</tr>
<tr>
<td>11:30-11:50</td>
<td>TA06</td>
<td>Single Drop Electrochemistry on a Screen-Printed Electrode</td>
<td>Charuksha Walgama, Oklahoma State University</td>
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#### Materials and Polymer Chemistry - Session 1 (S111)

<table>
<thead>
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<th>Session</th>
<th>Title</th>
<th>Presenter(s)</th>
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<tbody>
<tr>
<td>9:30-10:00</td>
<td>TM01</td>
<td>Silicon-Based Hyperbranched Polymers</td>
<td>Petar R. Dvornic, Pittsburg State University</td>
</tr>
<tr>
<td>10:00-10:20</td>
<td>TM02</td>
<td>General Mechanism of Glycerol Polymerization into Polyglycerol in Alkaline Catalysis</td>
<td>Mihail Ionescu, Pittsburg State University</td>
</tr>
<tr>
<td>10:20-10:40</td>
<td>TM03</td>
<td>Flexible Polyurethane Foams from Glycerin Polyols</td>
<td>Ivan Javni, Pittsburg State University</td>
</tr>
<tr>
<td>10:50-11:10</td>
<td>TM04</td>
<td>Hyperbranched Polyols From Biodiesel</td>
<td>Zoran Petrovic, Pittsburg State University</td>
</tr>
<tr>
<td>11:10-11:30</td>
<td>TM05</td>
<td>Dynamics of Methyl Methacrylate Segments in Poly(styrene-co-methyl methacrylate) in Bulk and on Silica</td>
<td>Madhubhashini Maddumaarachchi, Oklahoma State University</td>
</tr>
<tr>
<td>11:30-11:50</td>
<td>TM06</td>
<td>Surfactant Catalysis: An Unusual Approach to Room-Temperature Radical Polymerizations</td>
<td>Tan Zhang, Oklahoma State University</td>
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</tbody>
</table>

#### Materials and Polymer Chemistry - Session 2 (S110)

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Presenter(s)</th>
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<tbody>
<tr>
<td>9:30-9:50</td>
<td>TM07</td>
<td>Syntheses of Indium (III) tetrachlorophenoxy Phthalocyanine Complex for use in Organic based Solar Cells</td>
<td>Casey Williamson, East Central University</td>
</tr>
<tr>
<td>9:50-10:10</td>
<td>TM08</td>
<td>Electrochemical Properties of Graphene Absorption</td>
<td>Yushi Zang, University of Central Oklahoma</td>
</tr>
<tr>
<td></td>
<td>TM09</td>
<td>Consequences of Steric Mismatch on Tg Composition Dependence for</td>
<td></td>
</tr>
</tbody>
</table>
10:10-10:30  Poly(4-hydroxystyrene)/Hydroxypropylcellulose Blends  
Carl L. Aronson, Northeastern State University

10:50-11:10  TM11 Experimental and Molecular Dynamics Simulation Studies of Adsorbed Polymers on Silica  
Hamid Mortazavian, Oklahoma State University

11:10-11:30  TM12 Middle and End labelled PMMA-d3: The Effect of Chain Ends on Polymer Dynamics  
Ugo N. Arua, Oklahoma State University

11:30-11:50  TM13 Quantifying the Wettability of Porous Membranes  
Lida Baghernejad, University of Tulsa

Organic Chemistry (S109)

9:30-9:50  TO01 SubPc-ZnPorphyrin conjugates - Synthesis, Characterization and Properties  
Lakshmi Chockalingam Kasi Viswanath, Oklahoma Baptist University

9:50-10:10  TO02 Reaction of 2-Caboxybenzaldehyde with Amines and Trimethylsilyl Cyanide or Triethyl Phosphite Catalyzed by OSU-6  
Richard A. Bunce, Oklahoma State University

10:00-10:30  TO03 Novel Bio-Based polyols for Rigid Polyurethane Foams  
Nelson Elbers, Pittsburg State University

10:50-11:10  TO04 Synthesis and Evaluation of Second Generation Flex-Het Scaffolds Against the Human Ovarian Cancer A2780 Cell Line  
Krishna Kumar Gnanasekaran, Oklahoma State University

11:10-11:30  TO05 Using Solution and Solid-State NMR to Determine the Structure, Dynamics and Interactions of Biologically Relevant Membrane Proteins  
Gabriel A. Cook, Oklahoma State University

11:30-11:50  TO06 Modular Synthesis of Amphiphilic Networks with Guest-Host Capabilities  
Mathis Hodge, Oklahoma State University

Environmental Chemistry (S120)

9:30-9:50  TE01 The removal of Arsenic Species from Fruit Juice and other Aqueous Samples using Iron Oxyhydroxides  
Travis Reed, Oklahoma State University

9:50-10:10  TE02 Selectivity and Kinetic Behavior of Heavy Metals and Radionuclides on Supported Ion Exchange Adsorbants  
Wesley T. Honeycutt, Oklahoma State University and *Xplosafe

10:10-10:30  Analysis of Leaching of Dibutyl Phthalate from a Commercial Faucet Hose into Water using Solid Phase Microextraction (SPME) and Gas Chromatography Mass Spectroscopy (GC MS)  
Dalton Lewis and Juliette Chisam, University of Central Oklahoma, Edmond North High School

Chemical Education (S120)

10:50-11:10  TC01 STEM Educational Enhancement Initiative by High School Students  
A.K.Fazlur Rahman, Oklahoma School of Science and Mathematics
**Instrumental Analysis as a Sophomore Course**
Michael Jordan, Oklahoma Baptist University

**Changing the Perspective of Waste: Neutralization of BZ Reaction for an Exciting “Green” Undergraduate Chemistry Lab**
Madison J. Duckwall, Southwestern Oklahoma State University

**Organometallic Chemistry (S111)**

1:00-1:20 TR01 Recent Advances in Cyano-Substituted Pyrazoles and Cyanoscorpionates Chemistry
Lava Raj Kadel, Wichita State University

1:20-1:40 TR02 Effect on Properties of Ion Exchange Resins due to use of Filming Amines in Condensate Systems
Ahmedul Kabir, Oklahoma State University

**Nanoscience (S110)**

1:00-1:20 TN01 Investigation of the Acid-Base Behavior of Cr-Based Mesoporous Nanoparticles: An in situ FT-IR Study
Dilip Paul, Pittsburg State University

1:20-1:40 TN02 Artifact Detection and Image Correction for Scanning Tunneling Microscope Images
Mitchell P. Yothers, The University of Oklahoma

1:40-2:00 TN03 High Performance Supercapacitors based on Hydrothermally Synthesized Iron Oxide Nanoparticles
Felipe D. Souza, Pittsburg State University

**Inorganic Chemistry**

1:00-1:20 TI01 Zinc 2-Oximinocarboxylates for Low-Temperature Preparation of Nanocrystalline Zinc Oxides
Evangeline Rukundo, Oklahoma State University

1:20-1:40 TI02 Liquid Metal Carboxylates for Synthesis of Bimetallic Oxide
Allen Apblett, Oklahoma State University

**Physical and Computational Chemistry (S120)**

1:20-1:40 TP01 A Spectroscopic View of Water/Zeolite Interactions
Kuizhi Chen, Oklahoma State University

1:40-2:00 TP04 Investigation of the Stability of Silver Halide Films On the Atomic Scale
Jesse Phillips, University of Tulsa

**Poster Session (corridor outside S103)**

GA01 Sandwich Immunoassay for Insulin Detection by a Surface Plasmon Microarray Imager
Jinesh Niroula, Oklahoma State University

GB01 Opioids and Non-Steroidal Anti-Inflammatory Drugs
Allen Chen, Oklahoma School of Science and Mathematics

GE01 Arsenic remediation
Zach Brown, Oklahoma State University
GE02  New Fluorescent Method for The Detection of Scale Inhibitors Using Inorganic Complexes
Reem Mofleh Alshamrani, Oklahoma state university

GI01  Synthesis and Characterization of Vanadium Based Precursors for Metal Orthovanadates
Asma Alothman, Oklahoma State University

GM01  Glycerin Based Polyurethane Cast Elastomers
Nikola Bilic, Pittsburg State University

GM02  Non-Isocyante Polyurethanes from Soybean Oil and Aromatic Cyclic Carbonates
Olivera Bilic, Kansas Polymer Research Center, Pittsburg State University

GM03  Simple NMR Experiments Reveal the Influence of Chain Length and Chain Architecture on the Crystalline/Amorphous Interface in Polyethylenes
Arifuzzaman Tapash, Oklahoma State University

GM04  Synthesis of Eumelanin-inspired polyindoles
K. A. Niradha Sachinthani, Oklahoma State University

GM05  Synthesis and characterization of Eumelanin-inspired ethynylene-linked polymers
Santosh Adhikari, Oklahoma State University

GN01  Infrared Studies of Photochemistry of Adsorbed Species over Semiconducting Nanoparticles
Dilip Paul, Pittsburg State University

GN02  Application of Silver, Gold, and Platinum complexes in Medicine
Tina Wu, Oklahoma School of Science and Mathematics

GO01  Kinetics of Thermal Reaction of Model Alkyne-azide Compounds
Jian Hong, Pittsburg State University

GO02  Synthesis and Biological Activity of New Dihydrophthalazine-Appended 2,4-Diaminopyrimidines
Nagendra P. Muddala, Oklahoma State University

GO03  Efficient Synthesis of 1,3,4-Oxadiazoles Promoted by NH4Cl
Krishna Kumar Gnanasekaran, Oklahoma State University

GP01  DFT study of the dissociative adsorption of chlorobenzene and 1,2-dichlorobenzene on Si(100)
Eric Butson, Oklahoma State University

UA01  Optimization of Solid Phase Microextraction Gas Chromatography-Mass Spectrometry Parameters for The Analysis of Onion (Allium cepa) Vapors
Z. M. Willems, Tabor College

UA02  Effect of the Percent Composition of Fatty Acid Methyl Esters of Biodiesel on the Cloud Point of the Solution
T. J. Entz, Tabor College

UB01  Cys-Cys Crosslinking Blocks Iron Transport in E. coli Through an Outer Membrane Channel
Kyle J. Moore, Cameron University

UC01  Organic Compounds as Glaucoma and Antiulcer Agents
Brian Dick, Oklahoma School of Science and Mathematics

UC02  Development of a Laboratory Component for the Advanced Inorganic Chemistry Course at East Central University
UM01  **Flexible High Performance Energy Storage Device for High Temperature Applications**
John Candler, Pittsburg State University

UM02  **Charge Transport Mechanism in Photodiode based on Phthalocyanine/n-Silicon for photovoltaic applications**
Tyler Elmore, Pittsburg State University

UM03  **Solvent Diffusion from Polymer Solutions with Lyotropic Liquid Crystalline Capability**
Carl L. Aronson, Northeastern State University

UM04  **Graphene based high performance electrode for flexible energy storage devices**
Ashley Jimenez, Pittsburg State University

UM05  **Heavy Metal Electrochemical Sensors**
Wil Sisson, Pittsburg State University

UM06  **Electrical properties and DFT studies of Copolymers from 3-phenyl[5]ferrocenophane-1,5-dimethylene and various para substituted phenylmaleimides**
Henry Thomas, Pittsburg State University

UM07  **Biosensor Studies with Copolymers from Vinylferrocene and 4-Vinylpyridinium**
Raymond B. Westby, Pittsburg State University

UN01  **Low Temperature FT-IR Studies of Acetaldehyde on GaInTiO$_2$: Role of Acid-Base Sites**
Juan Gaucin, Pittsburg State University

UP01  **Reactions of Manganese Oxides at High Temperatures**
Laura G. Asaro, East Central University

HS01  **The Ebola Virus Glycoprotein: An Essential Envelope Protein for the Life Cycle of Ebola Virus**
Bill Lackamp, Sierra Loveland, Adrian McAfee, Marie Montague, Daniel Munguia, Keaton Wilber, James Foresman, and Irene Zegar, Pittsburg High School SMART Team

TO08  **Development of a Microscale Procedure for the Suzuki Coupling Reaction to Produce 4-Acetylbiphenyl from Phenylboronic Acid and 4-Bromoacetophenone**
Amanda Purtell, Oral Roberts University

TO07  **Synthesis of Ethyl 4-(3-Fluorophenyl)-6-Methyl-2-Oxo-1,2,3,4-Tetrahydropyrimidine-5-Carboxylate and Its Effect on the Proliferation Rate of HEK T293 Fibroblast Cells**
Zachary Youmans, Oral Roberts University

TP02  **Scaled Quantum Mechanical Scale Factors for Vibrational Calculations using Alternate Polarized and Augmented basis sets with the B3LYP Density Functional Calculation Model**
William B. Collier, Oral Roberts University

TP03  **Matrix Isolation of Anserine in Argon at 18 K Using Infrared Spectroscopy**
Matthew C. Stricker, Oral Roberts University
Abstracts

TA01  **Enhancement of Catalytic Features of Heme Proteins Attached to Magnetic Nanoparticles**
Presenter: Gayan Premaratne
Authors and Affiliation: Gayan Premaratne, Ryan Matlock, Trey Sunday, Sadagopan Krishnan
Department of Chemistry, Oklahoma State University - Stillwater

Catalytic efficiency of covalently conjugated heme proteins to magnetic nanoparticles (MNP) and the effect of scale up of this miniature MNP-protein bioreactor are examined in this study. Conjugates of MNP-heme protein were prepared by using carbodiimide chemistry to covalently link model myoglobin protein to polyacrylic functionalized MNP (100 nm hydrodynamic diameter). The MNP amount used was scaled up in the order of 1, 5 and 10 times to evaluate the protein-catalyzed reaction product yields, reusability and stability of the conjugates prepared. The peroxidase like activity of myoglobin was utilized in evaluating the oxidation of 2,2-azino-bis(3-ethylbenzothiazoline-6-sulfonate) (ABTS) as the color developing dye. The reusability tests of MNP-protein conjugate were performed by reusing the conjugate repeatedly with fresh reactant solution and the stability was checked for 7 and 14 days storage in phosphate buffer solution (pH 7.4). The ABTS oxidation product was quantified using UV/Visible spectrophotometry. Five and ten fold scaling up of MNP amounts resulted in two fold and four fold increment in products. Conjugation proved extensive stability for even 4 months in comparison to a solution of myoglobin in buffer. Thus, MNP conjugation with catalytic biomolecules opens up a new direction in developing volume-efficient, miniaturized, and highly economical green bioreactors.

TA02  **pH Indicator to Enhance Surface Plasmon Resonance Imaging Detection of Weak Acids**
Presenter: Zainab Al Mubarak
Authors and Affiliation: Zainab Al Mubarak, Gayan Premaratne, and Sadagopan Krishnan
Chemistry Department, Oklahoma State University, Stillwater

pH is an essential parameter in biological, medical and industrial applications. Monitoring the pH level in biological fluids reflects the abnormal conditions in human body. During industrial food processes, it is important to monitor the pH to maintain the desired flavor. Therefore, highly sensitive, rapid and continuous measurement of pH is desirable. Many pH sensors have been invented such as pH electrode, optical pH sensors that are based on absorption or fluorescence of pH indicator dyes. Surface plasmon resonance microarray imager (SPRI) is a unique technique, which is highly sensitive to the change in refractive index of a gold surface in contact with a dielectric medium, and the measurements can be performed in a few seconds. Change in color of an analytical reaction reveals the corresponding change in refractive index, thus SPRI can be used in combination with pH indicator to measure the pH of different concentrations of acids and bases. Here in, we illustrate that SPRI can be used to detect the refractive index change of pH indicator such as methyl red at different pH values with high sensitivity, which can be considered as a new method for measuring pH of precious, less abundant samples such as body fluids in a clinical setting.

TA03  **Morphologies Controlled Synthesis of CoS2 for Enhanced Electrochemical Properties**
Presenter: E. Alqurashi
Authors and Affiliation: E. Alqurashi, Ram K. Gupta
Department of Chemistry, Pittsburg State University

Nanostructured CoS2 was synthesized by a facile hydrothermal method. The effect of growth parameters such as solvent and presence of surfactants on the size and morphology of CoS2 was investigated. It was observed that these variations could provide CoS2 with range of sizes, shapes and morphologies. The nanostructured CoS2 were structurally and electrochemically characterized. The structural characterizations were performed using X-ray diffraction (XRD) and scanning electron microscopy (SEM). The electrochemical measurements were performed in a standard three electrode cell containing a platinum wire as a counter electrode, a saturated calomel electrode as a reference electrode and CoS2
on nickel foam as a working electrode. The potential application of these materials for supercapacitors was tested using cyclic voltammeter and galvanostatic charge discharge method. It was observed the specific capacitance of CoS2 depends on its morphology and electrolyte. The maximum specific capacitance of 335 F/g was observed in 3 M NaOH electrode. The electrochemical stability of these electrodes was also investigated. The results suggest that CoS2 could be used as an electrode material for fabrication of supercapacitor devices.

TA04 Synthesis of Reduced Graphene Oxide and the Effects of Adsorption of Organic Compounds by Structure
Presenter: Tye Chapman
Authors and Affiliation: Tye Chapman, John Bowen, Barry Lavine
Chemistry, University of Central Oklahoma, Oklahoma State University
A low-cost synthesis of graphene, derived from the Hummers and Offeman method was developed. A commercial grade graphite lubricant was exfoliated with concentrated acid, oxidized by permanganate to produce graphene oxide (GO). This was then reduced using hydrazine hydrate to produce graphene. Products were analyzed using Raman Spectroscopy and SEM. Both species were used to observe the effect of structure of various organic species on absorption in water. The adsorption was analyzed by difference using solid phase micro extraction (SPME) and gas chromatography mass spectrometry.

TA05 Development of a Microfluidic Immunological Assay for the Detection and Identification of Bluetongue Virus and EHDV Induced Antibodies in Serum.
Presenter: Mary Tappert
Authors and Affiliation: Mary Tappert, John Bowen, Jane Jarshaw, Robert Brennan
Chemistry and Biology, University of Central Oklahoma
This study describes the development and testing of a microfluidic immunological assay that combines lateral flow assay and microfluidic paper-based analytical device designs for the purpose of detecting and identifying antibodies in serum from sheep exposed to Bluetongue Virus and/or EHDV. Initial design research was done using BSA and anti-BSA to mimic the actual target antibody/antigens. The final assay design will use BTV or EHDV proteins as antigen and animal serum as primary antibody, with antigen-antibody binding detected by a fluorophore- or gold nanoparticle-labeled secondary antibody. We here describe the stepwise optimization of antigen binding, antibody flow, and complex detection in a microfluidic system.

TA06 Single Drop Electrochemistry on a Screen-printed Electrode
Presenter: Charuksha Walgama
Authors and Affiliation: Charuksha Walgama, Matt Gallman, Anuruddha Pathirana and Sadagopan Krishnan
Chemistry, Oklahoma State University
Bulky instruments for electrochemical biosensor applications generate many practical disadvantages when the instant detections have to be taken in laboratory conditions or in fields. Conventional Electrochemical detecting techniques comprised with cells with three electrode components, which need large volumes of electrolytes and analytes. Here the same three-electrode system is fabricated on a disposable screen-printed electrode, which needs only about 20 μl of analyte sample for the electrochemical detection. In our preliminary studies, we detected a few biologically important compounds of NADH, Ascorbic acid and Nicotine in micro molar concentrations on multi-walled carbon nanotube modified screen-printed electrodes. Voltametric oxidation signals were recorded under non-enzymatic conditions. Therefore the single drop analysis on tiny electrode strips may open up new analytical methods to be more cost effective, portable and decentralized. Furthermore, the surface modifications can extensively improve the sensitivity and the selectivity of the analytical approach, which leads to development of novel high throughput off-lab portable screening systems for various biologically and environmentally important samples.
Silicon-Based Hyperbranched Polymers
Presenter: Petar R. Dvornic
Authors and Affiliation: Petar R. Dvornic, Chemistry Department, Pittsburg State University

Hyperbranched polymers are unique among polymer molecular architectures for their combination of very high density of functionality, low viscosity and easy synthesis for a given molecular weight and composition. They can be made by monomolecular and bimolecular non-linear polymerization and until present hydrosilylation and nucleophilic substitution of silanols have played the most important roles as the synthetic pathways of choice. A variety of different silicon-containing compositions have been reported, among which polycarbosilanes, poly(carbosilane-siloxanes), polysiloxanes, poly(silarylene-siloxanes) and poly(fluorocarbosilane-siloxanes) have attracted the most attention. Of these, the first mentioned ones are even commercially available. In this talk, synthetic pathways to preparation of some of hyperbranched silicon-containing polymers will be discussed together with their properties and demonstrated or possible applications. Attention will also be paid to some organic hyperbranched polymers which are siliconized to gain useful new properties.

General Mechanism of Glycerol Polymerization into Polyglycerol in Alkaline Catalysis
Presenter: Mihail Ionescu
Authors and Affiliation: Mihail Ionescu, Dragana Radojcic, Zoran Petrovic
Kansas Polymer Research Center, Pittsburg State University

Polymerization of glycerol into polyglycerol with basic catalysts (NaOH, KOH, NaOCH3, KOCH3, CaO etc.) is an old reaction. Unfortunately the mechanism of this unusual reaction, with the formation of ether bonds, was not understood very well. Recent developments proved that the “key” of this reaction is the transformation of glycerol into glycidol followed by the ring opening addition of formed glycidol to the various hydroxyl groups from the reaction system. This mechanism explains the formation of linear and branched polyglycerols only, but does not explain the formation of cyclic polyglycerols. We demonstrated that other similar compounds such as triethanolamine or trimethylolpropane, with the same catalysts, do not polymerize, but 1,2,6-hexanetriol polymerizes into poly(1,2,6 hexanetriol). We concluded that the structural “key” of this reaction is the 1,2-glycol structure and not only glycerol but diglycerol, triglycerol or polyglycerols having terminal 1,2 glycol structures can generate terminal epoxy groups which react with hydroxyl groups from the reaction system. Cyclic polyglycerols are formed by intramolecular reaction of these terminal epoxy groups with a hydroxyl group from the same molecule. It appears that the transformation of 1,2-glycols in epoxy groups in the presence of alkaline catalysts is a general reaction and we identified many other compounds having 1,2-glycol structure which polymerize. The resulting polyether polyols, of high functionality, are very interesting new intermediates for the preparation of polyurethanes (rigid foams, coatings, adhesives, etc.).

Flexible Polyurethane Foams from Glycerin Polyols
Presenter: Ivan Javni
Authors and Affiliation: Ivan Javni, Olivera Bilic, Vladislav Jaso and Nikola Bilic
Kansas Polymer Research Center, Pittsburg State University

Flexible polyurethane slab stock foams are used as cushioning materials in furniture, transportation, and packaging. They are made from petrochemical polyols of molecular weight 3000 – 4000, toluene diisocyanate, water as blowing agent and catalyst. This work examined the feasibility of replacing part of the petrochemical polyol with a high bio-content glycerin based polyol. Glycerin is a by-product of biodiesel production and can be used in foams in small amounts as the crosslinker. However, for the use as the base polyol it must be chemically modified. We have developed a process for conversion of glycerin into high bio-content polyols that have hydroxyl numbers in the range of 50 – 60 and viscosity below 5 Pa.s, which is considered acceptable for this kind of application. Glycerin based polyol was included up to 30 parts in blend with petrochemical polyol. The foams were prepared using a blend of polyols, toluene diisocyanate, catalysts, and surfactants, commonly used in polyurethane foams, with water as the blowing agent. The formulations were adjusted to produce foams of density of around 30
kg/m³. Testing of foams included open cell content, mechanical and thermal properties. The foams with glycerin polyol reached the desired open cell content of over 90%, but displayed decreased foam hardness, rebound resilience, and compression, tensile and tear strength. They can be used in cushioning, packaging, energy absorbing or similar applications as replacement for pure petrochemicaly based polyurethane foams.

**TM04  Hyperbranched Polyols From Biodiesel**  
Presenter: Zoran Petrovic  
Authors and Affiliation: Zoran Petrovic, Ivan Javni  
Kansas Polymer Research Center, Pittsburg State University  
Structure of polyols to a large degree determine PU properties. For flexible applications such as coatings and foams, molar mass of polyols must be above 3000 g/mol and functionality greater than 2. Polyester polyols prepared from fatty acids (FA) are of special interest due to availability of fatty acid methyl esters (bio-diesel). Methyl esters must be functionalized by introducing hydroxyl groups in order to create polymerizable hydroxyl fatty acids. The objective of this work was to create polyols of high molecular weight and low viscosity starting from soybean bio-diesel. The method involved hydroformylation of soybean oil fatty acid methyl esters and self- polymerization to desired OH and viscosity. Polyols were characterized by GPC/lights scattering and viscosity measurements. Foams with up to 60% of biobased polyols in the mixture with petrochemical polyols were prepared and tested.

**TM05  Dynamics of Methyl Methacrylate Segments in Poly(styrene-co-methyl methacrylate) in Bulk and on Silica**  
Presenter: Madhubhashini Maddumaarachchi  
Authors and Affiliation: Madhubhashini Maddumaarachchi, Frank D. Blum  
Chemistry, Oklahoma State University  
Segmental dynamics of adsorbed samples of poly(methyl methacrylate) homopolymer and poly(styrene-co-methyl methacrylate) copolymers on silica was studied using deuterium quadrupole-echo NMR spectroscopy. Homopolymer and copolymer samples, with different methyl methacrylate (MMA) percentages, were synthesized by free radical polymerization and the adsorbed samples were prepared by solution deposition using toluene. Spectra were collected at different temperatures, below and above the glass transition temperature, for the bulk and the adsorbed samples of homo- and copolymers. The effect of the adsorption and the copolymer composition on the segmental dynamics of the above systems was evaluated. Surface adsorbed homo- and copolymers showed significant spectral differences from bulk. The solid-state 2H NMR spectra of surface adsorbed polymers indicated that copolymers had larger fraction of bound MMA units compared to the homopolymer revealing MMA units preferentially find their way to the silica surface.

**TM06  Surfactant Catalysis: An Unusual Approach to Room-Temperature Radical Polymerizations**  
Presenter: Tan Zhang  
Authors and Affiliation: Tan Zhang, Frank D. Blum  
Chemistry, Oklahoma State University  
Conducting radical polymerizations at room temperature not only reduce energy consumption, but also have potential applications in biomedical materials. Surfactant catalysis was found to be an efficient approach to lower the activation energy for thermal initiators to decompose, consequently initiated radicalpolymerizations at lower temperatures. The efficiency of surfactant catalysis was affected by several factors, such as the types and the concentrations of surfactant the nature of monomers and the viscosities. With proper design of the surfactant catalysis systems, the rates of surfactant catalyzed radical polymerizations at 21 °C were found to be much larger than that of regular free radical polymerizations at 60 °C when the same concentrations of initiator AIBN were used.
Syntheses of Indium (III) Tetrachlorophenoxy Phthalocyanine Complex for use in Organic based Solar Cells

Presenter: Casey Williamson
Authors and Affiliation: Casey Williamson, Dane Scott
Chemistry, East Central University

This presentation discusses the synthesis of a new Indium (III) tetrachlorophenoxy phthalocyanine complex for use in an organic based solar cell. The microwave synthesis of Indium (III) phthalocyanine is a simple two-step process. This method allows for a decreased reaction time. The initial step of reacting 3,5 dimethoxyphenol with 4,5 dichloro-1,2dicyanobenzene was carried out using Na2CO3 and DMSO as the solvent. The mixture was microwaved for a total of eight minutes. The product, 4-Chloro-5-(3,5dimethoxyphenoxyphthalonitrile), was then washed with cold deionized water and ethanol. The previous product was reacted with InCl3 using N, N DMAE as a solvent and microwaved for 11 minutes. After the synthesis a modified chromatography method was used to purify the compound using 10% chloroform/90% ethanol. The compound was added drop wise to the ITO/TIO2 slide. A second slide consisting of quasi solid conducting electrolyte based on polyacrylonitrile was layered on an aluminum slide. The two slides were then pressed together with clips. Current and Voltage were measured under 160W AM 1.5 radiation. These results will be discussed in comparison with a previous system based on copper phthalocyanine tetrasodium salt.

Electrochemical Properties of Graphene Absorption

Presenter: Yushi Zang
Authors and Affiliation: Yushi Zang, John Bowen, F. Albahadily
Chemistry, University of Central Oklahoma

Reduced graphene oxide was prepared and formed into a specially constructed form with electrodes on either end. Conductance and current were observed as phthalate esters were adsorbed onto the surface.

Consequences of Steric Mismatch on Tg Composition Dependence for Poly(4-hydroxystyrene)/Hydroxypropylcellulose Blends

Presenter: Carl L. Aronson
Authors and Affiliation: Carl L. Aronson, William T. Brewer
Department of Natural Sciences, Northeastern State University

An investigation of phenolic functional group accessibility in hyperbranched poly(4-hydroxystyrene) (PHS-B) is presented. The phase behavior and extent of hydrogen bonding in blends of either PHS-B or linear PHS with hydroxypropylcellulose (HPC), a complimentary Lewis basic polymer, were calculated from glass transition temperature (Tg) enhancements measured using differential scanning calorimetry (DSC) techniques. The effects of local steric screening and overall steric mismatch as well as the thermodynamic competition between inter-molecular and intra-molecular hydrogen bonding are discussed with respect to the observed miscibility and compositional dependence of blend Tg. An extension to literature equations applicable to conventional symmetric Tg composition dependence is presented in order to model asymmetric Tg composition dependence utilizing a coalescence concentration point. Furthermore, the effect of varying the Lewis base linear polymer molecular weight on the hydrogen bonded PHS-B fraction is discussed respect to the free energy of mixing polymers from Flory-Huggins theory. PHS-B/HPC blend data helped begin to establish a new molecular architecture-functional group accessibility property relationship for use with the design of functionalized hyperbranched synthetic macromolecular targets.

Experimental and Molecular Dynamics Simulation Studies of Adsorbed Polymers on Silica

Presenter: Hamid Mortazavian
Authors and Affiliation: Hamid Mortazavian, Christopher J. Fennell, and Frank D. Blum
Chemistry, Oklahoma State University

Temperature-modulated differential scanning calorimetry (TMDSC) of adsorbed poly(vinyl acetate) (PVAc) and poly(methyl methacrylate) (PMMA) on silica has been performed to probe the effects of
polymer adhesion. Although a broadened, two component transition has been reported for poly(methyl methacrylate) (PMMA) adsorbed on silica, three different regions of thermal activity were observed for PVAc. At low adsorbed amounts, the onset of segmental motion occurred at temperatures significantly higher (tightly-bound) than glass-transition temperature (Tg) of the bulk polymer. With increasing the adsorbed amounts, two other regions were found at temperatures slightly higher (loosely-bound) and slightly lower (Mobile component) than the Tg of bulk PVAc. The tightly-bound amount and the difference between the transition of tightly-bound and bulk-like polymer for adsorbed PMMA on silica was found to be higher than that for adsorbed PVAc. Using molecular dynamics simulations, we investigated the dynamical behavior of oligomer chains to provide insight on the interactions and structure of polymers adsorbed on silica. The dynamics and structure of these oligomers were analyzed near the silica surface, in the bulk-like polymer region and the polymer/air interface. The interactions between polymers and substrate have been quantified as the number density of carbonyl and alcoxy groups of polymers as a function of the radial distance from the silica surface. The silica surface modified the polymer structure at the interface and polymer chains formed three different layers evidenced by changes in the density profile of polymers. The strength of the intermolecular interactions were characterized by energy pair distribution of pairs of molecules (silanol groups of silica surface and side chain of polymers).

TM12 Middle and end labelled PMMA-d3: the effect of chain ends on polymer dynamics
Presenter: Ugo N. Arua
Authors and Affiliation: Ugo N. Arua, Frank D. Blum
Chemistry, Oklahoma State University
Poly(methyl methacrylate) (PMMA) block copolymers with deuterated segments were synthesized using atom-transfer radical polymerization with activators generated by electron transfer (AGET-ATRP) mediated by an iron catalyst. The polymer samples prepared had deuterated middle and end segments. These polymers were used to observe differences between the dynamics of the different segments of PMMA in bulk using solid state deuterium NMR. The implications to the behavior of these polymers when adsorbed will also be discussed.

TM13 Quantifying the Wettability of Porous Membranes
Presenter: Lida Baghernejad
Authors and Affiliation: Lida Baghernejad, Dr. Erin Iski
Department of Chemistry and Biochemistry, University of Tulsa
Materials with special wettability towards certain liquids are highly demanded for various industrial, environmental and biological applications. Such materials are designed and developed by many methods and in numerous structural forms. Porous membranes are among the most versatile materials with special wettability. Besides chemical composition, the surface structure of a porous membrane is highly effective on its wettability. The size, geometry and interconnectivity of the pores in a porous membrane significantly influence the wettability of the membrane. Therefore, determining the wettability of porous membranes is not as straightforward as quantifying the wettability of smooth solid surfaces. For instance, droplet contact angle measurement, which is a common technique for quantifying the wettability of many materials, is not very reliable for determining the wettability of porous materials. The present project focuses on reviewing, investigating and further understanding the fundamental concepts of quantifying the wettability of porous membranes. Moreover, it is intended to clarify the parameters that influence the wettability of porous membranes and develop techniques that are more precise and accurate in measuring the wettability of porous materials. Such investigations are of crucial for applications where porous substances with selective wettability are required.
TO01  **SubPc-ZnPorphyrin conjugates - Synthesis, Characterization and Properties**  
Presenter: Lakshmi Chockalingam Kasi Viswanath  
Authors and Affiliation: Lakshmi Chockalingam Kasi Viswanath, Kenneth D. Berlin, Laura D Shirtcliff, Sadagopan Krishnan, Nisha V Handa  
Chemistry, Oklahoma Baptist University  
In the recent years, the field of organic solar cells have challenged scientists in various aspects. A great deal of research has been invested towards improving the efficiency of solar cells by not only collecting the solar energy throughout the entire solar spectrum, but also in the effectual conversion of solar energy into resourceful chemical energy. As a means to achieve highly soluble donor –acceptor conjugates covering a broad range of the solar spectrum, and with increased efficiency of solar energy conversion, the construction of dyads and triads comprised of porphyrin and subphthalocyanine units has been established. A covalently linked B-O bond in the axial position can act as the electron donor and acceptor pair. Our research focusses on the synthesis of a set of SubPc-Porphyrin dyads and triads by the nucleophilic substitution reaction of hydroxyl-containing meso-substituted porphyrins and a good electron acceptor, dodecafluorosubphthalocyanine. The photophysical and electrochemical studies reveal the strong coordination existing between the two macrocycles. The synthesized ZnP-SubPc conjugates are expected to find applications in artificial photosynthetic system and various molecular electronic devices.

TO02  **Reaction of 2-Caboxybenzaldehyde with Amines and Trimethylsilyl Cyanide or Triethyl Phosphite Catalyzed by OSU-6**  
Presenter: Richard A. Bunce  
Authors and Affiliation: Richard A. Bunce, Baskar Nammalwar, Nagendra P. Muddala, Meaghan Murie  
Department of Chemistry, Oklahoma State University  
Reaction of 2-carboxybenzaldehyde with amines and trimethylsilyl cyanide or triethyl phosphite in the presence of OSU-6 catalyst gives high yields of (±)-3-oxoisooindoline-1-carbonitriles or (±)-diethyl 2-substituted (3-oxoisoiindolin-1-yl)phosphonates, respectively. The reaction has broad scope and is successful with most amines. The reaction with trimethylsilyl cyanide can be tuned to give the nitrile or the corresponding carboxamide product. Less reactive anilines, however, show divergent reactivity in the case of cyanide addition, while the reaction proceeds smoothly with triethyl phosphite. The two reactions will be presented and the unique reactivity of anilines will be discussed in mechanistic terms.

TO03  **Novel Bio-Based polyols for Rigid Polyurethane Foams**  
Presenter: Nelson Elbers  
Authors and Affiliation: Nelson Elbers, M. Ionescu, Ram K. Gupta  
Department of Chemistry, Pittsburg State University  
Beta-caryophyllene and alpha-phellandrene are two naturally-occurring alkenes which were used in this study to synthesized novel bio-based polyols. These polyols were used for the preparation of polyurethane rigid foams. A photochemical thiol-ene reaction was employed using beta-caryophyllene and alpha-phellandrene in combination with 1-thioglycerol and 2-mercaptoethanol to synthesize polyols with functionality of 3 and 4 depending on the molar equivalents of 1-thioglycerol and 2-mercaptoethanol. The synthesized polyols have been characterized using gel permeation chromatography, FT-IR, viscosity, and hydroxyl number. The synthesized polyols were successfully used for preparation of rigid polyurethane foams which contained 50% commercial polyol (Jeffol SG-360) and 50% of the synthesized bio-based polyols from this study. These polyurethane foams were characterized for mechanical property, closed cell content, apparent density, morphology, thermal stability and glass transition temperature. In addition to the foams mentioned above, polyurethane foams which contained 100% bio-based polyol were also produced and characterized in this study. Properties for these foams in each of the areas mentioned previously, concerning foams, were comparable to the properties of Jeffol SG-360 polyurethane foam, which served as an industrial reference. The goal is to assess these foams’ potential use for various applications such as thermal insulation of freezers, pipes, storage tanks, and buildings.
TO04  Synthesis and Evaluation of Second Generation Flex-Het Scaffolds Against the Human Ovarian Cancer A2780 Cell Line
Presenter: Krishna Kumar Gnanasekaran
Authors and Affiliation: Krishna Kumar Gnanasekaran, D. M. Benbrook, B. Nammalwar, E. Thavathiru, R. A. Bunce and K. D. Berlin
Department of Chemistry, Oklahoma State University
A structure activity relationship study was carried out on second generation Flex-Het compounds incorporating a 4-atom acrylamide linker between the two aromatic rings. Various substitutions on the terminal aromatic ring were explored and compound activity was compared to the parent Flex-Het compound, SHetA2 (NSC721689), which has a 3-atom thiourea linker and a nitro substituent on the terminal ring. Biological activity was measured using a cytotoxicity assay of the human A2780 ovarian cancer cell line treated with a range of compound concentrations.

TO05  Using solution and Solid-State NMR to Determine the Structure, Dynamics and Interactions of Biologically Relevant Membrane Proteins
Presenter: Gabriel A. Cook
Authors and Affiliation: Gabriel A. Cook, Chemistry, Oklahoma State University
Nuclear magnetic resonance spectroscopy (NMR) continues to improve as a method for elucidating physical properties of biological molecules. In the past, several aspects of NMR have limited its ability to be used as a widely applicable method for characterizing membrane proteins. Obviously, the size of the protein and its time correlation has been a major hurdle to overcome as we seek information about the larger subset of these macromolecules in lipid environments. The use of nanodisks and macrodisks allow us to take advantage of both solution and solid-state NMR to make measurements that give us relevant information about large membrane proteins in a bilayer environment. The latest developments in solid-state NMR, namely the use of rotational diffusion, allow us to make precise measurements of bond vector orientations for the calculation of a high-resolution 3D structure of membrane proteins. Two groups of proteins that we are applying these improved methods to are viroporins and glycoproteins. Information about the structure, dynamics and interactions of these important membrane proteins gained from NMR spectroscopy will be used to characterize their function and, in some cases, be used in the development of drugs targeting the disease causing forms of these biomolecules.

TO06  Modular Synthesis of Amphiphilic Networks with Guest-Host Capabilities
Presenter: Mathis Hodge
Authors and Affiliation: Mathis Hodge, Gaumani Gyanwali, Cameron Villines, and Jeffery L. White Oklahoma State University
Cyclodextrin (CD) functionalization can result in a diverse collection of amphiphilic compounds, with possible uses in drug delivery or drug recovery from waste streams, energy applications, biomedicine, and consumer products. Previously, CD functionalization with alkyl groups has been achieved using alkyl halide reagents involving concentrated NaOH reagents, followed by strong acid neutralization. To date, we have synthesized functionalized CD’s using a simple one-pot synthetic route involving dilute NaOH as the main reagent. Simple routes for macromolecular functionalization of CD cores to generate cross-linked networks have been demonstrated in which the CD rings are connected via aliphatic short chains. The more recent research has extended the basic synthetic methodology to generate macromolecular networks that contain polyethylene glycol (PEG) linkers between CD cores. In the resulting amphiphilic network structure the hydrophobic CD cavity has been maintained with a hydrophilic polymer matrix present.
Synthesis of Ethyl 4-(3-Fluorophenyl)-6-Methyl-2-Oxo-1,2,3,4-Tetrahydropyrimidine-5-Carboxylate and Its Effect on the Proliferation Rate of HEK T293 Fibroblast Cells

Presenter: Zachary Youmans
Authors and Affiliation: Zachary Youmans, William Ranahan, Lois Ablin
Oral Roberts University

In a multicomponent Biginelli reaction, Ethyl 4-(3-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate was synthesized under aqueous conditions from 3-fluorobenzaldehyde, urea, and ethyl acetoacetate. The compound was tested in several concentrations to assess the efficacy as an anti-proliferation agent in HEK T293 fibroblast cells. Results of the assay showed that two concentrations had an inhibitory effect on the cells.

Development of a Microscale Procedure for the Suzuki Coupling Reaction to Produce 4-Acetylbiphenyl from Phenylboronic Acid and 4–Bromoacetophenone

Presenter: Amanda Purtell
Authors and Affiliation: Amanda Purtell, Lois Ablin
Department of Biology and Chemistry, Oral Roberts University

A microscale procedure for the microwave-assisted synthesis of a Suzuki reaction product was developed for an undergraduate green organic chemistry laboratory experiment. Using palladium acetate as a catalyst, 4-bromoacetophenone and phenylboronic acid were combined under aqueous, basic conditions to produce 4-acetylbiphenyl. The CEM MARS™ Microwave System was used to synthesize the compound in various reduced scale modifications. Results of all scaled-down procedures were consistent with an average yield of 66%; products were characterized by physical properties and by FTIR and NMR spectroscopy.

The Removal of Arsenic Species from Fruit Juice and Other Aqueous Samples Using Iron Oxyhydroxides

Presenter: Travis Reed
Authors and Affiliation: Travis Reed, Allen Apblett
Chemistry, Oklahoma State University

Contamination of arsenic species have been found in various natural water systems and widely sold foodstuffs. These contaminants can have ill effects on human health, especially, on the very young. Arsenic contamination in juice has been given quite a bit of attention and even causing an action limit of 10 ppb to be put into place by the FDA to match that for potable water set by the EPA. The development of materials that can be used for removal of arsenic from these products is of importance to help allow for safer drinking for communities world-wide. Nanocrystalline iron and zinc oxyhydroxides and their solid solutions have been shown to uptake arsenic from various aqueous real life samples. These materials have the benefit being easy to synthesize by the low temperature decomposition of the metal pyruvic acid oxime salts leading to the only by-products being small volatile organic fragments and the metal oxide. This study will discuss the treatment of arsenic contaminated samples and fruit juice by iron/zinc oxyhydroxides.

Selectivity and Kinetic Behavior of Heavy Metals and Radionuclides on Supported Ion-Exchange Adsorbants

Presenter: Wesley T. Honeycutt
Authors and Affiliation: Wesley T. Honeycutt, Evgenii B. Kadossov*, Allen Apblett, Nicholas F. Materer
Chemistry, Oklahoma State University and *Xplosafe

The removal of radionuclides by selective concentration from seawater is an especially attractive goal since oceans contain valuable materials, although at low concentrations. Radionuclide sources include natural abundance and seepage plus that which is due to industrially generated wastewater streams and nuclear incidents. Challenges include the selectivity required for the low concentrations, high material volumes, and high ionic strengths. To address these problems, a recently available supported ion-
exchange adsorbent was determined by kinetic assay to be selective for uranium from simulated seawater. These assay were also preformed for neodymium, lead, cobalt, strontium, cadmium, cesium, copper, thorium, barium, chromium, and nickel adsorbates, chosen due to either their presence in common wastewater streams or as surrogates for more exotic radionuclides. The adsorbent was also tested using groundwater and lake water, each doped with analyte ions. Analysis of the data revealed properties about the exchange mechanism regarding the Langmuirian growth of the analytes on the adsorbent and leaching during subsurface migration by target ions. Under simulated conditions, the test material was able to concentrate heavy ions on the surface of the exchange interface with particular selectivity for uranium..

TE03 Analysis of Leaching of Dibutyl Phthalate from a Commercial Faucet Hose into Water using Solid Phase Microextraction (SPME) and Gas Chromatography Mass Spectroscopy (GC MS)
Presenter: Dalton Lewis and Juliette Chisam
Authors and Affiliation: Dalton Lewis and Juliette Chisam, Erin Brooks, Justin Westhover, Thomas Briscoe, John Bowen, F. Albahadily
Chemistry, University of Central Oklahoma, Edmond North High School
Various Phthalate Esters are used as plasticizers in commercial plastics and are known to leach into drinking water. Some are also implicated as endocrine disruptors. For this study, a common flexible plastic faucet hose was purchased from a hardware store, and analyzed using SPME-GCMS using an internal standard. Timed samples of deionized water were exposed to the hose, and quantitated for dibutyl phthalate concentration. Several internal standards were synthesized and used for this study.

TC01 STEM Educational Enhancement Initiative by High School Students
Presenter: A.K.Fazlur Rahman
Authors and Affiliation: A.K.Fazlur Rahman, Stormy Perry, Tomorrow Denton, Varun Enamuri, Julie Zhu, Maddyson All good, Mary Loveless, Jackie Pham, Jency Koshy, Kobby Wiafe, Jane Chin, Joseph Gao
Oklahoma School of Science and Mathematics
As part of our STEM education enhancement program at the Oklahoma School of Science and Mathematics to promote Chemistry education to elementary schools across the State of Oklahoma we have launched a "Science is Fun" program to teach science 4th, 5th and 6th grade students by the 11th, 12th grade students. This program was funded for a year by Dreyfus Foundation. In all these demonstrations we have used power point presentations, visual teaching using molecular models and science experiments to entertain and teach the students basic scientific concepts. Each class session was for about 50-60 mins. Most classes were held in the school auditorium to accommodate 120-150 students. Two - four OSSM students were involved in each teaching session. Fourteen OSSM student’s taught over one thousand elementary school students during the year.

TC02 Instrumental Analysis as a Sophomore Course
Presenter: Michael Jordan
Authors and Affiliation: Michael Jordan,
Oklahoma Baptist University
Instrumental Analysis has generally been taught as a senior-level course. In the current curriculum, however, students begin using instruments (especially spectrometers) early in their 4-year program. With the traditional approach, they use these instruments for 2-3 years before being taught what these instruments do and how they work. An alternate approach is to teach the most common spectroscopic techniques in the sophomore year and then follow up with less common instruments during the junior/senior level class. This sophomore-level class at OBU teaches the fundamental principles, spectrometer design, and interpretation of typical spectra for electronic, infrared, and nuclear magnetic resonance spectroscopies.
**TC03  Changing the Perspective of Waste: Neutralization of BZ Reaction for an Exciting “Green” Undergraduate Chemistry Lab**
Presenter: Madison J. Duckwall
Authors and Affiliation: Madison J. Duckwall, Tami A. Martyn, PhD
Department of Chemistry and Physics, Southwestern Oklahoma State University

In an effort to be environmentally friendly or “green” in our undergraduate labs, the products from one reaction have been used as the starting materials for a new experiment. This reaction follows the common Belousov-Zhabotinsky (BZ) Oscillating Reaction, which has highly acidic waste, a manganese indicator as well as aqueous and organic components. Neutralizing the extremely acidic waste from the BZ reaction with 6 M NaOH and NaHCO3 causes some unique phenomenon. Addition of BZ waste to NaOH causes a violent reaction heard across the room. With the added base, the solution goes from colorless to brown due to the oxidation of manganese ions in solution. Then as the sodium bicarbonate was added, CO2 produced through the reaction formed bubbles protruding 4.5 cm into the solution as well as over 15 cm above the solution. The reaction continued longer and more vigorously than sodium bicarbonate reacting with sulfuric acid or the acidic BZ waste alone. The BZ waste had a -0.02 pH, indicating the free hydrogen ion concentration. The total hydrogen ion concentration was 7.32 M as determined through titration, indicating the large quantity of protonated acids within the solution. NMR of the precipitate formed during the reaction confirms the presence of malonic acid. This experiment is extremely useful in a classroom because it builds on qualitative observation skills and is exciting, the kind of exciting that sparks people to become fascinated with chemistry. But most importantly, everything needed for the reaction is already present after performing the BZ reaction.

**TR01  Recent Advances in Cyano-Substituted Pyrazoles and Cyanoscorpionates Chemistry**
Presenter: Lava Raj Kadel
Authors and Affiliation: Lava Raj Kadel, David M. Eichhorn
Department of Chemistry, Wichita State University

For several years, our research group has been working with cyano-substituted pyrazoles and polypyrazolylborate ligands, also called cyanoscorpionate ligands. In the past we have reported the synthesis of 3,4-disubstituted pyrazoles with CN substituent at the fourth position of the ring. We have reported several sandwich, half-sandwich, inverted-sandwich and polymeric complexes of metals such as Fe, Ni, Co, Mn, Cu, Ag and Mo with the scorpionate ligands synthesized from 3,4-disubstituted cyanopyrazoles. Recently we have also been able to develop new 3,4,5-trisubstituted pyrazoles with CN substituents at the fourth position of the ring. Herein we report our recent developments in the field of cyanoscorpionates made from tri-substituted cyanopyrazole.

**TR02  Effect on Properties of Ion Exchange Resins due to Use of Filming Amines in Condensate Systems**
Presenter: Ahmedul Kabir
Authors and Affiliation: Ahmedul Kabir, Allen Apblett
Chemistry, Oklahoma State University

In condensate systems, filming amines are added to feedwater to coat and protect surfaces against corrosion but the properties and performance of polishing ion exchange resins can be affected as a result. To investigate the effect of exposure, two commercial filming amines and three other amines were used with four cation exchange resins and two anion exchange resins including two of those in powdered form. The resins properties in standard, exposed and regenerated forms were measured; LCMS, fluorometric analysis and salt splitting experiments were performed as well. According to the results of the study, filming amine uptake was higher for cation exchange resins as compared to the anion exchange resins. Decrease in exchange capacity was found for most resins and regeneration did not achieve a complete recovery of the resin properties. Absorption of amines and their presence after regeneration were confirmed by LCMS and fluorescence results.
Investigation of the Acid-Base Behavior of Cr-Based Mesoporous Nanoparticles: An in situ FT-IR Study

Presenter: Dilip Paul
Authors and Affiliation: Dilip Paul, Tanner Cheney, Juan Gaucin
Chemistry, Pittsburg State University

A novel approach was used to synthesize mesoporous Al-MCM and Cr-doped AlMCM material and these materials were characterized by UV, XRD and other techniques. Earlier investigators predicted their potential use for decomposition of toxic organic compounds. Here in this study, FTIR spectroscopy was used to determine the acid-base properties of this material using CO and pyridine as probe molecules. Both Lewis and Bronsted acid sites were found to be present as determined by corresponding IR modes on surfaces. Adsorption of acetaldehyde was used as a model compound to understand the reactivity of the nanoparticles towards catalytic degradation. During adsorption at low temperature, the acetaldehyde molecule binds through H-bonding with surface --OH groups. In addition, a fraction of acetaldehyde adsorbed through Lewis acid sites- Cr (IV) and Al (III). The combination of both H-bonded and Lewis acid sites bound acetaldehyde underwent condensation reaction forming aldol which then dehydrated at elevated temperature forming 2-butenal. A fraction of adsorbed acetaldehyde underwent photodecomposition to CO2 during photooxidation at 273 K and 173 K. This oxidation involves photoactive acetyl radical and Cr ion. A variety of condensation products also identified using temperature programmed desorption during photochemical reaction.

Artifact Detection and Image Correction for Scanning Tunneling Microscope Images

Presenter: Mitchell P. Yothers
Authors and Affiliation: Mitchell P. Yothers, Lloyd A. Bumm
Homer L. Dodge Department of Physics & Astronomy, The University of Oklahoma

A complete description of the monolayer structure of alkanethiol self-assembled monolayers (SAMs) on Au(111), e.g. the position of each molecule, can in principle be extracted from molecularly-resolved scanning tunneling microscope (STM) images. Unfortunately the analysis is complicated by imaging artifacts, the most problematic of which are piezo hysteresis and sample drift. If these artifacts could be corrected, a wealth of information about the SAM structure could be accessed. The goal of our work is to access that information using a suite of image analysis tools we have been developing in MATLAB. We explain the origin the imaging artifacts and models for their characterization. Our strategy allows removal of these artifacts, while losing a minimum of structural information. Because the molecular unit cell dimensions are typically known very accurately from other measurements, viz. x-ray diffraction, the molecular lattice can serve as an internal standard and enable the imaging artifacts to be removed. We are particularly interested in categorizing the monolayer lattice registration between structural domain boundaries and across Au(111) substrate step edges. Additional metrics of the SAM order can then also be obtained, such as the translational and orientational order.

High Performance Supercapacitors based on Hydrothermally Synthesized Iron Oxide Nanoparticles

Presenter: Felipe D. Souza
Authors and Affiliation: Felipe D. Souza, Ram K. Gupta
Department of Chemistry, Pittsburg State University

A facile hydrothermal technique was used to synthesize nanostructured iron oxide. The synthesized iron oxide was characterized using various techniques. The X-ray diffraction analysis confirms that the magnetite (Fe3O4) phase of the iron oxide. There were no extra peaks other than peaks due to Fe3O4 were observed indicating phase purity of Fe3O4. Further, the morphology and average particle size of the synthesized iron oxide were investigated using scanning electron microscopy. The average particle size of these nanoparticles was about 65 nm. Magnetic properties of the hydrothermally synthesized Fe3O4 nanoparticles were studied in detail. The magnetization of the Fe3O4 nanoparticles was studied by varying applied magnetic field and temperature. The magnetic measurement reveals the ferromagnetic nature of the synthesized Fe3O4 nanoparticles at room temperature with coercivity and remanence magnetization of 98 Oe and 0.51 μB/molecule, respectively. In M vs T measurements, we observed
a transition around 120 K. The observation of such transition (Verwey transition) indicates the high quality and phase purity of the synthesized Fe3O4. Moreover, the Fe3O4 nanoparticles were electrochemically characterized for their potential application as an electrode for ultra-capacitors. The specific capacitance of 97 F/g at the current of 1 mA was observed with excellent cyclic stability. The obtained high specific capacitance, excellent cyclic stability and ferromagnetic behavior at room temperature suggest that this facile method could be used for the production of cost effective magnetic and environment friendly iron oxide nanoparticles for next generation supercapacitor devices.

**TI01  Zinc 2-oximinocarboxylates for Low-Temperature Preparation of Nanocrystalline Zinc Oxides**
Presenter: Evangeline Rukundo
Authors and Affiliation: Evangeline Rukundo, Allen Apblett
Chemistry, Oklahoma State University
Low-temperature decomposition of metal containing precursors offers the advantage of preparing nanocrystalline materials with high surface areas by avoiding sintering. Salts of 2-oximinocarboxylates are promising candidates for use as low-temperature precursors for metal oxide ceramics due to their thermal instability and ligand decomposition into volatile fragments. This study investigates the thermal decomposition of zinc 2-oximinocarboxylates with different ligand side chains (R–): C2H5, (CH3)2CH, (CH3)3C, C6H5, and C6H5CH2. The precursor compounds and the metal oxides produced were characterized by infrared, Raman, 1H and 13C NMR spectroscopy, thermal gravimetric analysis, X-ray powder diffraction, and X-ray crystallography. Obtained results show that the size and orientation of R– group influence the coordination mode adopted by the ligand around the zinc ion center resulting in unique hydration degrees and hydrogen bonds within each complex. The type of coordination mode and nature of bonding in these salts affect their decomposition behavior and pyrolysis temperature thereby conditioning properties of resulting pyrolysis products.

**TI02  Liquid Metal Carboxylates for Synthesis of Bimetallic Oxide**
Presenter: Allen Apblett
Authors and Affiliation: Allen Apblett, Galina Georgieva, Larry Reinhardt, and Edwin Walker
Chemistry, Oklahoma State University
Metal salts of the polyether carboxylate, 2-(2-(2-methoxyethoxy)ethoxy)acetate (MEEA), are liquids at room temperature and are excellent solvents for other metal salts making them flexible precursors for the preparation of ternary metal oxides. For example dissolving magnesium nitrate in Al(MEEA)2OH gave a liquid that when heated to 700˚C produced crystalline spinel, MgAl2O4. Furthermore, colloidal metal oxide nanoparticles could be suspended in the liquid metal carboxylates to produce processible liquids that can be used to make nanostructured mixed oxides and fibrous metal silicates and aluminates. It was found that decomposition of the nickel MEEA salt in a mixture with a granular iron oxide led to deposition of a uniform conformal coating of nickel oxide on the surfaced of the iron oxide particles. Calcining this mixture resulted in an unusual solid-state reaction in which the precursor material mushroomed into broccoli-like clusters of small particles.

**TP01  A Spectroscopic View of Water/Zeolite Interactions**
Presenter: Kuizhi Chen
Authors and Affiliation: Kuizhi Chen, Jarred Kelsey, Lu Zhang, Daniel Resasco, and Jeffery L. White
Chemistry, Oklahoma State University
Zeolites are solid acids used extensively in petrochemical processes and also in methanol-to-hydrocarbon chemistry. However, zeolite reactivity can be affected by water. We have found that water can either increase or suppress the alkane C-H bond activation depending on the water loading (ACS Catalysis 2014, 4, 3039). To better understand the mechanism of water influence, baseline information about water-zeolite interaction should be acquired. Here in this presentation, zeolite ZSM-5 with different Si/Al ratios are introduced with different loadings of water from both liquid and gaseous phase. The water loadings varies from 1 molecule/per unit cell to oversaturated. Different loadings of water in HZSM-5 exhibit different chemical shifts, ranging from ca. 8 ppm to ca. 4 ppm depending on loadings of water. In
conjunction with solid-state MAS NMR experiments, pulsed-field gradient NMR experiments are used to investigate the self-diffusion coefficients of water in zeolites.

**TP02 Scaled Quantum Mechanical scale factors for vibrational calculations using alternate polarized and augmented basis sets with the B3LYP density functional calculation model**

Presenter: William B. Collier
Department of Biology and Chemistry, Oral Roberts University

The Scaled Quantum Mechanical (SQM) method of scaling calculated force constants to predict theoretically calculated vibrational frequencies is expanded to include a broad array of polarized and augmented basis sets based on the split valence 6-31G and 6-311G basis sets with the B3LYP density functional. Pulay's original choice of a single polarized 6-31G(d) basis coupled with a B3LYP functional remains the most computationally economical choice for scaled frequency calculations. But it can be improved upon with additional polarization functions and added diffuse functions for complex molecular systems. The new scale factors for the B3LYP density functional and the 6-31G, 6-31G(d), 6-31G(d,p), 6-31G+(d,p), 6-31G++(d,p), 6-311G, 6-311G(d), 6-311G(d,p), 6-311G+(d,p), 6-311G++(d,p), 6-311G(2d,p), 6-311G++(2d,p), 6-311G++(df,p) basis sets are shown. The double d polarized models did not perform as well and the source of the decreased accuracy was investigated. An alternate system of generating internal coordinates that uses the out-of-plane wagging coordinate whenever it is possible; makes vibrational assignments via potential energy distributions more meaningful. Automated software to produce SQM scaled vibrational calculations from different molecular orbital packages is presented.

**TP03 Matrix Isolation of Anserine in Argon at 18 K Using Infrared Spectroscopy**

Presenter: Matthew C. Stricker
Authors and Affiliation: Matthew C. Stricker, Denesha D. Stover, William B. Collier
Department of Biology and Chemistry, Oral Roberts University

Anserine is a dipeptide-like compound of pharmaceutical interest, and partially known biological function in mammalian biochemistry. But exactly how it functions is still under scrutiny. This presentation presents the 18 K frozen argon matrix isolated FTIR spectrum of anserine. The molecule contains multiple functional groups for hydrogen bonding that cause strong polymerization making it difficult to study using normal infrared spectroscopy. This experiment presents the matrix isolated monomer, dimer spectrum of anserine. The resulting spectrum had major matches within the functional group regions that deviated by 10-15 cm⁻¹ from the B3LYP/6-31G(d) SQM scaled calculated frequencies. Because of the extensive perturbing hydrogen bonding in the solid phase, this would have been impossible to achieve with normally collected solid phase FTIR spectra.

**TP04 Investigation of the Stability of Silver Halide Films On the Atomic Scale**

Presenter: Jesse Phillips
Authors and Affiliation: Jesse Phillips, Abigail Lee, Heather Morgan, Lauren Jackson, Dr. Sanwu Wang, Dr. Erin Iski
Department of Chemistry and Biochemistry, University of Tulsa

In previous research completed by Iski et al., it was found that through specific electrochemical methods, a silver (Ag) monolayer could be formed on an Au(111) surface in an electrochemical environment in both a chloride-free and chloride-rich solution. The work done at Tufts University showed that, in a chloride-free environment, the Ag monolayer could be formed and atomically resolved; however, once removed from the cell, it could be completely removed via hydrogen flame annealing. Interestingly, in the presence of chloride, the same Ag monolayer was formed and was found to be extremely thermally stable after removal from the cell and was resistive to temperatures as high as 1,000 K. The atomic structure of these films can be studied with electrochemical scanning tunneling microscopy (EC-STM), which not only allows for atomic scale imaging of the surface layer within an electrochemical environment, but also facilitates the taking of cyclic voltammograms (CVs), which can be used to examine the redox behavior of the
systems. Despite many studies on these types of surface layers, very few publications have directly studied their extreme thermal stability. Since it is known that the stability of bulk metal halide structures decreases as the halogen ion increases in size, it would be interesting to examine the stability of 2D AgBr or AgI films in comparison to what has been determined for the AgCl film. In order to better understand the structures and stability, density functional theory (DFT) will also be used to look at the equilibrium coverage and the diffusion barrier of the halogens on the Ag monolayer. Using EC-STM and DFT, we plan to study the ways in which this remarkable stability is imparted to the single crystal surface under ambient conditions.

**GA01 Sandwich Immunoassay for Insulin Detection by a Surface Plasmon Microarray Imager**
Presenter: Jinesh Niroula
Authors and Affiliation: Jinesh Niroula, Zainab Al Mubarak, Charuksha Walgama, Sadagopan Krishnan
Chemistry, Oklahoma State University

According to the National Diabetes Statistics Report released on June 10, 2014, 29.1 million Americans had diabetes in 2012 of which, 21.0 million were diagnosed and 8.1 million undiagnosed. In 2010, diabetes was the 7th leading cause of death in the United States, as complications cause severe health problems, which may include diabetic retinopathy, kidney failure, heart attack, cardiovascular diseases, and others. It is therefore important to have early and continuous detection of insulin levels in blood serum to identify type 1 diabetes (level < 50 pM) and type 2 diabetes (level at the onset > 70 pM) [under fasting conditions]. The objective of this research is to develop a novel, ultra-sensitive sandwich immunoassay for insulin biomarker in serum samples by Surface Plasmon Resonance microarray imager (SPRI) as the detection method. Capture antibodies (Ab1) were attached to SPR gold chip, while magnetic particles (MP) were conjugated to secondary antibodies (Ab2) and different concentrations of insulin in human serum were captured to obtain MP-Ab2-Insulin bioconjugates. Similarly, buffer insulin samples were analyzed for comparison and understand the influence of serum matrix in the detection levels. Magnetic particles produce amplified SPR signals when Ab1 captures insulin from the bioconjugate samples.

**GB01 Opioids and Non-Steroidal Anti-Inflammatory Drugs**
Presenter: Allen Chen
Authors and Affiliation: Allen Chen and A.K.Fazlur Rahman, Department of Chemistry, Oklahoma School of Science and Mathematics

Painkillers work through a variety of functions, including prostaglandin inhibition and the activation of opioid receptors in the nervous system. Non-Steroidal Anti-Inflammatory Drugs are the most common, mainly inhibiting the action of cyclooxygenase enzymes, which are involved in provoking pyretic and inflammatory responses from the body. Since they all have a similar function, their side effects also share similarities, mainly arising from the inhibition of cyclooxygenase. Opioids, which are drugs that interact with the nervous system and affect the brain’s response to pain, are the other main category of painkillers. Since they actually interact with the brain, they can be extremely addictive and habit-forming, but also can sometimes be the only form of effective treatment available for a patient. The purpose of this paper is to investigate the link between the chemical structure of these molecules and their medical functions.

**GE01 Arsenic remediation**
Presenter: Zach Brown
Authors and Affiliation: Zach Brown, Allen Apblett
Chemistry, Oklahoma State University

Arsenic pollution in drinking water affects people all around the world. There are many negative health effects associated with the consumption of arsenic, including skin, liver and kidney damage. Arsenic occurs in the environment naturally from the leaching of arsenic containing minerals and occurs through some anthropogenic causes like the semiconductor industry and through the use of wood preservatives. We have synthesized several mixed Fe:Zn hydroxide materials by altering the Fe:Zn ratios. These materials have a high affinity for arsenic, and can be used in different aqueous solutions. This talk will
discuss how the kinetics and capacities of these materials change as the ratio of Fe:Zn is varied. The possibility of these materials being useful for the remediation of other heavy metals will be explored.

**GE02 New Fluorescent Method for The Detection of Scale Inhibitors Using Inorganic Complexes**

Presenter: Reem Mofleh Alshamrani  
Authors and Affiliation: Reem Mofleh Alshamrani, Allen Apblett  
Chemistry, Oklahoma State University  

Scale formation in oil and gas industry has been known to be an essential problem that can cause low flow efficiency and blocking of the equipment walls. Scale inhibitors are one of the several techniques that have been used to eliminate or control the scale depositions. The scale inhibitors are one of the most used methods to control the scale in the oil field with a very small effective amount that can perfectly remove the scale. Our goal in this project is to determine and investigate the efficient concentrations of scale inhibitors to get the concentration that is needed of it in the oil field by a novel spectrofluorometric method using different inorganic complexes. In this project, we used environmentally friendly scale inhibitors to investigate by spectrofluorimetric method by synthesis of inorganic complexes such as Al-Morin. The addition of the scale inhibitor to the fluorescent systems led to immediate fluorescence inhibition, which was proportional to their amounts.

**GI01 Synthesis and Characterization of Vanadium Based Precursors for Metal Orthovanadates**

Presenter: Asma Alothman  
Authors and Affiliation: Asma Alothman, Allen Apblett  
Chemistry, Oklahoma State University  

Mixed metal vanadium oxides/hydroxides have emerged as an important materials with wide range of remarkable properties and possible application in catalysts, Li-ion batteries, chemical sensors, etc. This study reports the synthesis of mixed metal vanadium precursors and their conversion to the corresponding metal orthovanadates. The precursors were synthesized via aqueous reaction of vanadyl oxalate with the metal oxides or hydroxides. Infrared spectroscopy, thermal gravimetric analysis, and X-ray powder diffraction were employed to characterize the precursor compounds and the corresponding metal orthovanadates. The influence of the reaction time, temperature and the precursor’s stoichiometry on the decomposition temperature, particle size, and surface area of resulting metal orthovanadates was investigated. In addition, potential catalytic applications of the synthesized metal orthovanadates will be reported.

**GM01 Glycerin Based Polyurethane Cast Elastomers**

Presenter: Nikola Bilic  
Authors and Affiliation: Nikola Bilic, Ivan Javni, Zoran Petrovic  
Kansas Polymer Research Center, Pittsburg State University  

Glycerin, a by-product of bio-diesel production, is a suitable, abundant and inexpensive renewable raw material for the synthesis of polyols for polyurethanes. There are different methods to modify glycerin, such as oligomerisation, esterification, etc. We have developed a cost effective method for polyol production from glycerin that meets the requirements for a broad range of polyurethanes. This successfully optimized chemical route provided a range of polyols suitable for producing polyurethane elastomers, coatings, adhesives, binders, foams, etc. As anticipated, these polyols had viscosity, hydroxyl number and other characteristics typical of commercial polyols used for these various applications. A series of polyurethane cast resins were prepared from mixtures of glycerin-based polyols and petrochemical polyols, in varying ratios, with diphenylmethane diisocyanate (MDI). Petrochemical polyols that were used in this work had molecular weights 3000 – 4000. The resulting polyurethane cast resins were characterized by differential scanning calorimetry, dynamical mechanical analysis, thermomechanical analysis, thermogravimetric analysis and mechanical testing. All samples had high mechanical strength along with other properties desirable for applications such as casting materials, coatings, adhesives, sealants, etc. The goal to successfully replace a portion of the typical petrochemical polyol from the polyurethane formulation with a high bio-content glycerin-based polyol was realized.
GM02  Non-Isocyante Polyurethanes from Soybean Oil and Aromatic Cyclic Carbonates
Presenter: Olivera Bilic
Authors and Affiliation: Olivera Bilic, Ivan Javni and Zoran S. Petrovic
Kansas Polymer Research Center, Pittsburg State University
The reaction products of polyols and isocyanates are polyurethanes. These materials are among the most broadly used class of polymers, due to their excellent physical and mechanical properties. However, the reduced use of the highly toxic and hazardous isocyanate starting materials continues to be a major concern for those seeking to protect the environment and reduce the health hazards of personal exposure. An alternative approach is the production of isocyanate-free polyurethanes. One possible earth-friendly method for their preparation involves the reaction of cyclic carbonates with multifunctional amines. Non-isocyanate polyurethanes, synthesized from cyclic carbonates and amines, are interesting new polymeric materials. An important plus for this technology is its utilization of carbon dioxide, an inexpensive and environmentally friendly monomer. These new polyurethanes, with hydroxyl groups present in their chain structure, display enhanced properties relative to those prepared via the classical isocyanate route. Using this approach, we have developed non-isocyanate soy-based polyurethanes for applications as adhesives, coatings and foams. The current research has focused on increasing the rigidity and glass transition temperature (Tg) of non-isocyanate polyurethanes based on carbonated soybean oil (CSBO) and various diamines. The resulting modified CSBO non-isocyanate polyurethanes display improved mechanical and thermal properties when compared with non-modified ones.

GM03  Simple NMR Experiments Reveal the Influence of Chain Length and Chain Architecture on the Crystalline/Amorphous Interface in Polyethylenes
Presenter: Arifuzzaman Tapash
Authors and Affiliation: Arifuzzaman Tapash, Paul J. DesLauriers; Jeffery L. White
Chemistry, Oklahoma State University
The distribution of polyethylene (PE) chain segments between the crystalline, non-crystalline, and interfacial morphological regions is an old question that continues to intrigue the polymer science community. Simple solid state NMR experiments described here reveal that even in the case of linear PE, four distinct chain components may be resolved and reliably quantified. The amounts of rigid crystalline chains in all trans conformations, non-crystalline/amorphous trans-gauche chains undergoing essentially isotropic reorientation, mobile all-trans chains (termed mobile trans), and less mobile non-crystalline chains (termed constrained amorphous) can be quantified by simple 13C NMR experiments on solid polymer samples. A version of the EASY background suppression pulse sequence (Jaeger and Hemmann, Solid State Nuclear Magnetic Resonance, 2014, 57-58, 22), modified to eliminate transient Overhauser effects, is used to obtain all of the data in a single experimental acquisition. Using a broad range of well-characterized linear metallocene PE’s, the method reveals that the constrained amorphous and the mobile all-trans fractions, i.e., the total interface content, increases essentially linearly with increasing Mw. Topologically modified PE’s, at similar Mw’s, that contain short-chain branches (SCB), long-chain branches (LCB), or long-chain branches with SCB’s (LCB+SCB), have significantly larger interfacial content per unit molecular weight, most significantly so for the LCB+SCB polymers. In total, the results suggest a tool to assess and facilitate large-scale design and control of interfacial morphology in polyethylenes and related properties.

GM04  Synthesis of Eumelanin-inspired polyindoles
Presenter: K. A. Niradha Sachinthani
Authors and Affiliation: K. A. Niradha Sachinthani, Toby L Nelson
Department of Chemistry, Oklahoma State University
Melanins are naturally occurring pigmented polymeric networks found in skin, hair, eye and brain of mammals. Eumelanin, a brown-black biopolymer, is the most common form of melanin, which is composed of 5,6-dihydroxyindole and 5,6-dihydroxyindole-2-carboxylic acids. It is known as photoprotective agent due to its high degree of conjugation, and extremely higher absorption of ultraviolet and visible radiation. Eumelanin biopolymers have also been proposed for optoelectronic and photovoltaic applications but isolation of natural eumelanin is a difficult task. Therefore, it is beneficial to
synthesize synthetic eumelanin materials, which mimics the natural pigment. Currently, we have synthesized an eumelanin-inspired indole core, methyl 4,7-dibromo-5,6-dimethoxy-N-methyl-1H-indole-2-carboxylate which can serve as a new building block for organic semiconductors. Here, we present our efforts toward the synthesis and characterization of eumelanin-inspired polyindoles using different cross coupling methods such as Suzuki Miyaura and Grignard Metathesis.

GM05  **Synthesis and Characterization of Eumelanin-Inspired Ethynylene-Linked Polymers**  
**Presenter:** Santosh Adhikari  
**Authors and Affiliation:** Santosh Adhikari, Niradha Sachinthani, Subhashini Selvaraju, Toby L. Nelson Chemistry, Oklahoma State University  
Melanins are naturally occurring pigment found in hair, eye, skin and brain of mammals. Eumelanin is a type of melanin which is responsible for the brown and black coloration and it has extremely high light absorption ranging from 200 to 600 nm in the electromagnetic spectrum. It is known to be a heterogeneous network, formed by two monomers 5,6-dihydroxyindole and 5,6-dihydroxyindole-2-carboxylic acid. In 1974, Eumelanin was established as an amorphous organic semiconductor with the work of Proctor and McGinness. Currently, we have synthesized a eumelanin-inspired indole core, methyl 4,7-dibromo-5,6-dimethoxy-N-methyl-1H-indole-2-carboxylate which can serve as a new building block for organic semiconductors. From this indole core, a series of small molecules have been synthesized with different alkynyl substituent at the 4, 7 - positions that alter the optoelectronic properties. Here, we will present the synthesis and characterization of eumelanin-inspired ethynylene-linked polymers.

GN01  **Infrared Studies of Photochemistry of Adsorbed Species over Semiconducting Nanoparticles**  
**Presenter:** Dilip Paul  
**Authors and Affiliation:** Dilip Paul  
Chemistry, Pittsburg State University  
The photooxidation of acetaldehyde and 2-CEES (2-chloroethyl ethyl sulfide) has been investigated over TiO2- based nanomaterial using molecularly sensitive-FTIR spectroscopy. Here the study involves the photochemical reaction of acetaldehyde over SrTiO3 nanomaterial and a mustard gas simulant, 2-CEES, over TiO2-SiO2 nanomaterial. The UV-Vis used irradiation in the range of 2.1 to 5.0 eV. It has been found that a large fraction of acetaldehyde undergo aldol condensation during dark oxidation forming crotonaldehyde. However, during exposure of UV-Vis light, a large fraction of aldehyde undergo extensive oxidation forming CO¬2 and other oxidized products. A similar oxidation of 2-CEES forming predominantly CO2 was noticed over TiO2-SiO2 nanomaterial indicating that titania-based nanomaterial could potentially be used for oxidation of toxic organics.

GN02  **Application of Silver, Gold, and Platinum complexes in Medicine**  
**Presenter:** Tina Wu  
**Authors and Affiliation:** Tina Wu and A.K.Fazlur Rahman, Department of Chemistry, Oklahoma School of Science and Mathematics  
In this presentation we summarize various usages of silver, gold, and platinum complexes and nanoparticles in medicine including some future perspective. Recent research data showed the versatility of metals in pharmacology and medicine. In medicine, metals are now used as complexes or as nanoparticles. When used as complexes, the compounds attach to various ligands in the body to serve targeted functions. Platinum complexes are used to treat cancer due to its ability to prevent the division of living cells. Silver complexes interrupt the ability of bacteria cells to form bonds which causes the bacteria to fall apart. While silver nanoparticles are relatively inert, gold nanoparticles were found to be effective, especially in the treatment of cancer.
**GO01 Kinetics of Thermal Reaction of Model Alkyne-azide Compounds**

Presenter: Jian Hong

Authors and Affiliation: Jian Hong, Dragana Radojčić, Djavan Hairabedian, Xianmei Wan, Zoran S Petrović; Kansas Polymer Research Center, Pittsburg State University

Alkynated and azidated octadecane, synthesized from 9-octadecane, were used as model compounds to study the kinetics of thermal Huisgen 1,3-dipolar cycloaddition. The kinetics study of model reaction is very helpful to understand the thermal polycycloaddition of alkynated and azidated vegetable oils whose main components are triglyceride containing aliphatic chains of 16-22 carbons. Three kinds of analysis methods (GPC, 1H NMR, and DSC) were used to study the kinetics. Detailed kinetic analysis revealed the reaction of alkynated and azidated octadecane needs 24 hours to reach 90% conversion at 100 °C. The reaction’s activation energy is 55 J/mol and the reaction order is 0.88.

**GO02 Synthesis and Biological Activity of New Dihydropthalazine-Appended 2,4-Diaminopyrimidines**

Presenter: Nagendra P. Muddala

Authors and Affiliation: Nagendra P. Muddala, B. Nammalwar, R. A. Bunce, K. D. Berlin, C. R. Bourne, E. W. Barrow and W. W. Barrow

Department of Chemistry, Oklahoma State University

The synthesis and biological activity of new substituted dihydropthalazine-appended 2,4-diaminopyrimidine dihydrofolate reductase inhibitors will be presented. These compounds are being developed to counter Bacillus anthracis as a potential bioterrorist threat.

**GO03 Efficient Synthesis of 1,3,4-Oxadiazoles Promoted by NH4Cl**

Presenter: Krishna Kumar Gnanasekaran

Authors and Affiliation: Krishna Kumar Gnanasekaran, Baskar Nammalwar, Maeghan Murie and Richard A. Bunce

Department of Chemistry, Oklahoma State University

An efficient and inexpensive approach to the synthesis of 2-substituted and 2,5-disubstituted 1,3,4-oxadiazoles from arylhydrazides and orthoesters is reported using catalytic NH4Cl. The conditions are mild, and thus, compatible with a variety of functional groups. The optimized reaction is performed using 30 mol% of NH4Cl in 100% EtOH and is generally complete within 1 h for non-aromatic orthoesters and 2-10 h for aromatic orthoesters. The reaction permits both electron-releasing and electron-withdrawing groups on the arylhydrazide substrate. Most products are formed in high yield and require only minimal purification. Compared with earlier reports, the current reactions proceed in shorter time and require less of the orthoester.

**GP01 DFT study of the dissociative adsorption of chlorobenzene and 1,2-dichlorobenzene on Si(100)**

Presenter: Eric Butson

Authors and Affiliation: Eric Butson, Qing Zhu, Nicholas F. Materer

Oklahoma State University

The dissociative adsorption of chlorobenzene and dichlorobenzene on Si(100) surface was modeled using density functional theory. A double and triple dimer cluster was used to represent the (100) face of silicon. Initial adsorption occurs by breaking one double bond on the phenyl ring and forming two new carbon-silicon bonds with the silicon dimer. For further dissociation to occur, the system must undergo a spin crossing process from the singlet electronic configuration to a higher energy triplet state. After this spin crossing event, the chlorine can then bond to the silicon surface. The possible mechanisms of dissociation are explored for both chlorobenzene and dichlorobenzene. The minimum energy crossing point for the spin crossing is found by minimizing the energy gradients between the two electronic states. The probability of spin crossing at the minimum energy crossing point is calculated, and the activation
energy for the process is determined. It is found that the activation energies for the spin crossings are small in comparison to the other steps in the proposed mechanisms.

UA01 Optimization of Solid Phase Microextraction Gas Chromatography-Mass Spectrometry Parameters for The Analysis of Onion (Allium cepa) Vapors
Presenter: Z. M. Willems
Authors and Affiliation: Z. M. Willems, N. E. Schmidt
Chemistry, Tabor College
Onion (Allium cepa) tissue was crushed and the juice collected in a test tube. A polydimethylsiloxane-divinylbenzene (DPMS-DVB) solid phase microextraction (SPME) fiber was then exposed to the vapor above the juice for 3.0 minutes. The fiber was then analyzed using GCMS. The injector temperature was varied for optimum results. At low injector temperatures the chemicals in the SPME did not properly desorb. At high injector temperatures the chemicals decomposed prior to entering the GC column. The column temperature was increased from 50°C to 190°C at 10°C/min. The transfer line temperature was not to be found critical for optimum results and was held constant at 275°C.

Some of the major chemicals found in onion vapor are: z-propanethiol-(S)-oxide, 2-methyl-2-pentenal, methyl propyl disulfide, dipropyl disulfide, propyl-1-propenyl disulfide and di-1-propenyldisulfide. We hypothesize that several of the disulfides were formed from the decomposition of thiosulfinates, although no thiosulfinates were observed.

Three different types of onions were analyzed using the new method. The onions were statistically different from one another based on the distribution of the chemicals observed. The main differences were found in the amounts of z-propanethiol-(S)-oxide, dipropyl disulfide and di-1-propenyldisulfide formed.

UA02 Effect of the Percent Composition of Fatty Acid Methyl Esters of Biodiesel on the Cloud Point of the Solution
Presenter: T. J. Entz
Authors and Affiliation: T. J. Entz, N. E. Schmidt
Chemistry, Tabor College
One of our country’s biggest issues is our dependence on fossil fuels. However, due to environmental and economic concerns, a market has been created in the search for alternatives. One of the most promising alternatives lies in the field of biofuels, specifically biodiesel.

However, one of the main hurdles for the mass commercial use of biodiesel is the temperature at which the liquid turns to a solid; its cloud point. The cloud point is based on the chemical composition of the fatty acid methyl esters (FAMEs) in the biodiesel which is determined by the type of feedstock used in the production of biodiesel.

In this research biodiesel samples were produced from a wide variety of fatty acid sources. The biodiesels were first analyzed for the composition of FAMEs using gas chromatography-mass spectrometry (GCMS) and then analyzed for cloud point using a thermometer and a water bath. From this data we have established a calibration curve to predict the cloud point of a sample of biodiesel based on its relative concentration of saturated FAMEs.

UB01 Cys-Cys Crosslinking Blocks Iron Transport in E. coli Through an Outer Membrane Channel
Presenter: Kyle J. Moore
Authors and Affiliation: Kyle J. Moore, Tiffany Cardell and Alex Fisher
Chemistry, Physics, and Engineering, Cameron University
Iron is utilized in metabolism, DNA replication and synthesis, and gene expression for all living organisms. Therefore, iron (III) acquisition is essential to living organisms. Since the availability of free iron is low, there are several systems in Gram-negative bacteria for obtaining iron from the environment or host organism (1). One system involves a typical TonB dependent outer membrane (OM) protein channel called FepA. FepA recognizes and transports the siderophore ferric enterobactin (FeEnt), which
coordinates an Fe(III) ion in the environment at low concentrations. FepA is a member of the porin family and contains 22 b-strands arranged in a barrel. FepA has a 150 amino acid N-terminal, globular domain within the barrel, suggesting that the N-terminal domain must undergo structural changes to allow the transport of FeEnt. To investigate these required changes, we created Cys mutants of FepA with either one or two Cys substitutions. These single and double Cys mutants were tested for their ability to transport FeEnt. While the single Cys mutants transported FeEnt similar to wild-type FepA, the double Cys mutants only transported FeEnt in the presence of a reducing agent. This result suggests that a disulfide bond prevented conformational changes in the N-terminal domain of FepA during FeEnt transport. These results taken with previous evidence support a model where the N-terminal domain remains in the b-barrel but rearranges for transport.

UC01 Organic Compounds as Glaucoma and Antiulcer Agents
Presenter: Brian Dick
Authors and Affiliation: Brian Dick, A.K. Fazlur Rahman
Chemistry, Oklahoma School of Science and Mathematics
Glaucoma is an eye condition that damages the optic nerve. Although initially asymptomatic, glaucoma leads to blindness. Current treatment for glaucoma includes the use of organic compounds such as Timolol, Bimatoprost (Lumigan), and travoprost (Travatan). For ulcer treatment organic compounds such as Cimetidine (Tagamet), Nizatidine (Axid) and Famotidine (Pepcid) are prominent. During the presentation structural aspect of these compounds and biological function will be discussed.

UC02 Development of a Laboratory Component for the Advanced Inorganic Chemistry Course at East Central University
Presenter: Cerina D. Stiles
Authors and Affiliation: Cerina D. Stiles, Dwight L. Myers
Chemistry, East Central University
The Chemistry Department at East Central University recently modified its advanced inorganic chemistry course to include a laboratory component. As an Honors component of the existing course, prospective laboratory procedures in the literature are being evaluated. Among other experiments, synthesis of boron nitride (BN), and synthesis of the yttrium barium copper oxide superconductor are being evaluated. While these are both well explored reactions, there are a variety of experimental procedures listed in the literature. These are being evaluated for their suitability in our laboratory. Efforts to date will be presented, along with an assessment of the feasibility of utilizing these experiments in the course.

UI01 Indium Complexes with Nitrogen and Sulfur Donor Ligands
Presenter: Michael T. Sullivan
Authors and Affiliation: Michael T. Sullivan, Nilmini Senaratne and David M. Eichhorn
Department of Chemistry, Wichita State University
Diagnostic imaging in radiopharmaceuticals has become a significant area of interest for indium research due to indium’s labeling ability in the body. However, indium compounds are typically unstable in the body, reacting with sulfur-containing proteins, which causes a buildup in the liver. Ligands containing nitrogen and sulfur donor atoms have been shown to aid in the stability of indium complexes due to their strong bonding abilities. Previous research in our lab has involved the use of 2,2'-dithiodibenzaldehyde (DTDB) in combination with ethylenediamine (en) to form the ligand N,N’-ethylenebis(thiosalicylideneimine) (tsalen). Tsalen has successfully been used to synthesize complexes with nickel, iron, and copper centers. In this paper, we report the synthesis of a stable indium compound, In(tsalen)(OAc), by the reaction of DTDB and ethylenediamine with indium(III) acetate, and the spectroscopic and crystallographic characterization of this complex. A side product of this synthesis, In(en)2(OAc)2, has also been crystallographically characterized. The indium complexes created may aid in the future development of radiopharmaceuticals.
UM01  Flexible High Performance Energy Storage Device for High Temperature Applications
Presenter:  John Candler
Authors and Affiliation:  John Candler, T. Elmore, R. K. Gupta
Pittsburg State University
A facile hydrothermal method has been used for the synthesis of cobalt molybdate (CoMoO4). It was observed that the morphology of CoMoO4 depends on growth conditions. Different morphologies such as cauliflower, brick and nano-sphere have been achieved. The proposed potential use of the CoMoO4 as an electrode material for flexible supercapacitor applications was examined by cyclic voltammetry (CV) and galvanostatic charge-discharge measurements. It was observed that the specific capacitance of the CoMoO4 depends on its morphologies. The specific capacitance of 169 F/g in 3M KOH at the current of 1 mA was observed for the nano-sphered CoMoO4. The specific capacitance was observed to depend on the type of electrolytes and showed the highest value of 259 F/g in 3M NaOH electrolyte. We have fabricated flexible supercapacitor device by sandwiching two electrodes separated by an ion transporting layer. The device shows no degradation in the capacitive properties on bending and shows improved stability with number of cyclic CV performance. The effect of temperature on the charge storage properties of the device was also investigated for high temperature applications. The specific capacitance of the device significantly increased when the operational temperature of the device was elevated from 10 to 70 oC. Hence, this work provides an ultimate facile method to synthesize morphologies controlled cobalt molybdates for the applications in next generation flexible energy storage devices which could drive more efficiently at higher temperature.

UM02  Charge Transport Mechanism in Photodiode based on Phthalocyanine/n-Silicon for photovoltaic applications
Presenter:  Tyler Elmore
Authors and Affiliation:  Tyler Elmore, John Candler, Ram Gupta
Pittsburg State University
Copper phthalocyanine (CuPc)/n-silicon junction was fabricated using thermal evaporator method. X-ray analysis of the CuPc film confirms the β-phase with preferred orientation along (100) direction. The crystallite size of the CuPc film was estimated using XRD data and observed to be about 12.6 nm. The current-voltage characteristics of Au/CuPc/n-Si/Au device was studied in dark and under illumination. The device shows diode characteristics. The diode parameters such as ideality factor, barrier height and series resistance were determined using different techniques such as conventional forward bias I -V characteristics, Cheung method and Norde’s function. A good agreement between the diode parameters calculated form these methods was observed. The analysis of the diode characteristics confirms that the transport mechanism of the Au/CuPc/n-Si/Au diode at the higher electric fields is governed by the space-charge-limited currents. The photoconducting behavior of the diode suggests that it can be used as a photosensor in optoelectronic applications.

UM03  Solvent Diffusion from Polymer Solutions with Lyotropic Liquid Crystalline Capability
Presenter:  Carl L. Aronson
Authors and Affiliation:  Carl L. Aronson, Brittney M. Rogers
Department of Natural Sciences, Northeastern State University
Thin films of poly(n-hexyl isocyanate) solutions were juxtaposed against air in a diffusion couple geometry at room temperature. The solvent was allowed to diffuse away and evaporate from the solution in a controlled manner. The diffusion couple geometry produced a uniform film for optical assessment of liquid crystalline potential between crossed polarizers. After an induction period, a stable microstructure developed in which the interior of the sample remained isotropic followed by a liquid crystalline band, with characteristic disclination defects and texture, followed by a crystalline band nearest to the external surface. The width of the total characteristic birefringent band was measured over time and provided information concerning the dynamics and trajectory of solvent transport and evaporation from the cover slip edge. The apparent solvent diffusion coefficient for each system was measured at room temperature as a function of initial polymer concentration. Consequences for concentrated biological macromolecular
systems possessing lyotropic capability are discussed with respect to the concentration dependence of solvent diffusion observed herein.

**UM04 Graphene based High Performance Electrode for Flexible Energy Storage Devices**

Presenter: Ashley Jimenez  
Authors and Affiliation: Ashley Jimenez, Elias Mitchell, Ram K. Gupta  
Department of Chemistry, Pittsburg State University  
With increasing demand for flexible electronics and energy storage devices, there is an urgency in developing materials which meet the requirements of flexibility and high performance. With this aim, we have developed graphene based materials which could be used as an electrode material for flexible, portable and highly-efficient power sources. We have synthesized highly porous hierarchical flexible nanosheets of NiCo2O4–graphene oxide (NiCo2O4–GO) on nickel foam by a facile electrochemical deposition method. The morphogenesis of the NiCo2O4–GO hybrid nanostructure based electrode exhibits hierarchical porous flexible nanosheet-like structures. The charge storage properties and stability of these materials were electrochemical tested. The cyclic voltammetry and galvanostatic charge–discharge measurements indicated high cyclic stability and power storage capacity. A very high specific capacitance of 1078 F/g at a discharge current of 1 mA with a great cyclic stability was observed. The high performance of these electrodes were due to their hierarchical porous nanosheet-like structure. Our results suggest that these electrodes could be used for flexible energy storage devices.

**UM05 Heavy Metal Electrochemical Sensors**

Presenter: Wil Sisson  
Authors and Affiliation: Wil Sisson, Charles J. Neef  
Pittsburg State University  
Heavy metal contamination is a significant problem environmentally due to the high toxicity associated with these metals. Various metals such as lead, cadmium, arsenic, and mercury have been accidentally released into the environment from mining operations. Detection and identification of heavy metals is essential for protecting people, as well as, protection of the environment. Currently, we are working with copolymers of the ferrocenophane diene with vinyl imidazole. Since imidazoles are known to interact with heavy metals, changes to the CV of the ferrocenophane repeat unit are anticipated. We will report the characterization and heavy metal testing of these novel ferrocene-imidazole copolymers.

**UM06 Electrical Properties and DFT Studies of Copolymers from 3-Phenyl[5]ferrocenophane-1,5-dimethylene and Various Para Substituted Phenylmaleimides**

Presenter: Henry Thomas  
Authors and Affiliation: Henry Thomas, Benjamin O. Tayo, and Charles J. Neef  
Pittsburg State University  
Ferrocene containing polymers continue to receive considerable attention due to their well understood chemistry and stable redox responses. Our research has focused on understanding the spatial arrangement and electrical properties of alternating copolymers from 3-phenyl[5]ferrocenophane-1,5-dimethylene with various para substituted phenylmaleimides. Cyclic voltammetry using these chemically modified electrodes with aqueous sodium perchlorate showed two redox waves indicating electronic interaction between the ferrocenyl and maleimide moieties. To understand the spatial arrangement of the monomers, first-principle studies using density functional study (DFT) was used to obtain the optimized geometries. DFT studies clearly showed the ferrocenyl moiety in close proximity to the maleimide moiety, suggesting that electronic interactions could result between these two moieties.

**UM07 Biosensor Studies with Copolymers from Vinylferrocene and 4-Vinylpyridinium**

Presenter: Raymond B. Westby  
Authors and Affiliation: Raymond B. Westby, Charles J. Neef  
Pittsburg State University
Ferrocene polymers have received considerable attention as redox mediators due to their well-behaved reversible oxidation and redox stability. In addition, ferrocene has been shown to be an effective mediator for electron transfer from the redox enzyme to the electrode substrate. In this research, we have focused on copolymers containing vinylferrocene and 4-vinylpyridinium for biological sensor applications. Chemically modified electrodes were prepared by solution casting these materials onto a platinum electrode for subsequent cyclic voltammetry studies using sodium perchlorate as the supporting electrolyte. In this study we examined various ratios of ferrocene to pyridinium and the effects of alkyl chain length of the pyridinium on sensor performance. Use of these materials in biosensors for the detection of dopamine or serotonin will be presented.

UN01 Low Temperature FT-IR Studies of Acetaldehyde on GaInTiO2: Role of Acid-Base Sites
Presenter: Juan Gaucin
Authors and Affiliation: Juan Gaucin, Dilip K Paul
Chemistry, Pittsburg State University
To determine the role of acid-base sites on GaInTiO2, acetaldehyde adsorption was examined at different temperatures using a specially designed ultra-high vacuum (UHV) infrared cell. The UHV cell is attached to vacuum manifold which is continually pumped by a 60 L turbomolecular pump and diaphragm roughing pump. It has been found that at 233 K, acetaldehyde adsorbed through hydrogen bonding to surface hydroxyl groups as well as through Lewis acid sites over pretreated GaInTiO2 surface with hydrogen to form alcohol on the surface in the form an ethoxy species. 2-butenal (crotonaldehyde) was formed as the product of aldol condensation reaction and an acetate species was observed due to oxidation of acetaldehyde. This suggests that the acid sites play a crucial role in catalyzing the condensation, oxidation, and reduction reactions with acetaldehyde.

UP01 Reactions of Manganese Oxides at High Temperatures
Presenter: Laura G. Asaro
Authors and Affiliation: Laura G. Asaro, Dwight L. Myers
Chemistry, East Central University
Modern superalloys contain a wide range of metals in trace quantities. Reactivity and compatibility of oxides with other materials and with each other plays a significant role in choice of materials for developing Thermal Barrier Coatings (TBCs) for use in combustion environments. We are currently studying the reactivity of manganese oxides under atmospheric conditions at temperatures ranging from 500 - 1500°C. Reaction couples consisting of manganese oxides in various oxidation states in contact with oxides such as silicon dioxide or titanium dioxide are being studied. Results to date for these studies will be presented.

HS01 The Ebola Virus Glycoprotein: An Essential Envelope Protein for the Life Cycle of Ebola Virus
Authors and Affiliation: Bill Lackamp, Sierra Loveland, Adrian McAfee, Marie Montague, Daniel Munguia, Keaton Wilber, James Foresman, and Irene Zegar, Pittsburg High School SMART Team
The recent Ebola virus outbreak can be traced to a two-year old boy from Guinea who died shortly after contracting the virus. This disease is associated with a severe hemorrhagic fever with a mortality rate of 50-90%. Currently, FDA-approved vaccines for humans are nonexistent, due in part to the virus’s high replication rate. The Ebola viral envelope Glycoprotein (GP) consists of two subunits, GP1 and GP2, and is believed to mediate host recognition, attachment to and entry into the host cell as well as provide protection from immune defenses. A pre-fusion crystal structure of GP bound to a human survivor antibody (KZ52) reveals that the three GP1 subunits are cradled by the α-helices of GP2 forming a Chalice-like assembly of a trimer of GP1-GP2 heterodimers. It is believed that the GP1 residues making up the putative receptor-binding site reside within the inner bowl of the Chalice. This is in contrast to the anti-parallel six-helical bundle that GP2 adopts in its fusion form. The structure also reveals that three KZ52 antibodies are attached to the outer bowl of the Chalice through multiple Hydrogen-bonding and van der Waals interactions. Contact points between KZ52 and GP include residues 505-514 and 549-556 of GP2, as well as residues 42 and 43 of GP1. Insight into the structure suggests that the neutralization activity of the antibody results from its tight binding to GP2, thus preventing GP2 from rearranging to its
fusion form. Furthermore, a fully glycosylated model of the pre-fusion GP structure reveals that a glycan cap and a mucin-like domain cloak the majority of the Chalice thus restricting access to the highly conserved receptor-binding site. The Pittsburg High School SMART TEAM used 3D technology to design the Ebola virus GP bound to a human survivor antibody in order to understand the link between its structure and the role it plays in the life cycle of the virus. It is believed that new insights gained from this structure will facilitate the development of effective vaccines against this deadly virus.

GB01 Opioids and Non-Steroidal Anti-Inflammatory Drugs
Presenter: Allen Chen
Authors and Affiliation: Allen Chen and A.K.Fazlur Rahman, Oklahoma School of Science & Mathematics
Painkillers work through a variety of functions, including prostaglandin inhibition and the activation of opioid receptors in the nervous system. Non-Steroidal Anti-Inflammatory Drugs are the most common, mainly inhibiting the action of cyclooxygenase enzymes, which are involved in provoking pyretic and inflammatory responses from the body. Since they all have a similar function, their side effects also share similarities, mainly arising from the inhibition of cyclooxygenase. Opioids, which are drugs that interact with the nervous system and affect the brain’s response to pain, are the other main category of painkillers. Since they actually interact with the brain, they can be extremely addictive and habit-forming, but also can sometimes be the only form of effective treatment available for a patient. The purpose of this paper is to investigate the link between the chemical structure of these molecules and their medical functions.

GN02 Application of Silver, Gold, and Platinum complexes in Medicine
Presenter: Tina Wu
Authors and Affiliation: Tina Wu and A.K.Fazlur Rahman, Department of Chemistry, Oklahoma School of Science and Mathematics
In this presentation we summarize various usages of silver, gold, and platinum complexes and nanoparticles in medicine including some future perspective. Recent research data showed the versatility of metals in pharmacology and medicine. In medicine, metals are now used as complexes or as nanoparticles. When used as complexes, the compounds attach to various ligands in the body to serve targeted functions. Platinum complexes are used to treat cancer due to its ability to prevent the division of living cells. Silver complexes interrupt the ability of bacteria cells to form bonds which causes the bacteria to fall apart. While silver nanoparticles are relatively inert, gold nanoparticles were found to be effective, especially in the treatment of cancer.

HS02 Molecular Docking Studies of the DNA Interaction of Pyrethroids
Presenter: Adrian McAfee
Authors and Affiliation: Adrian McAfee and Irene Zegar, Pittsburg High School and Pittsburg State University
Pesticides are widely used worldwide in the agricultural industry. This prompted many researchers to investigate possible links between their continuous human exposure and the increase in certain cancers and neurodegenerative diseases among farmers, which include lung cancer, leukemia, as well Alzheimer’s and Parkinson’s disease. For example, a cohort study conducted over an 8-year period (1993-2001) on more than 90,000 pesticide applicators and their spouses showed a significant lung cancer increase after eliminating risk factors such as cigarette smoking, age and other genetic factors. Furthermore, a study done on rat exposure to pyrethroids (a class of pesticides) shows significant lymphocyte DNA damage due to prolong exposure to certain pyrethroids. Moreover, high levels of pyrethroids have been shown to cause apoptosis and DNA fragmentation in vitro and in vivo. The mechanism of which pyrethroids induce their adverse effects has remained elusive. We believe that these molecules can potentially exert their biological effects through interaction with DNA. To investigate the validity of this hypothesis, we studied the DNA interactions of a host of pyrethroids and their cellular metabolites using molecular docking calculations. Our calculations show that these
compounds bind DNA with equilibrium binding constants as high as $2 \times 10^6$. $K_a$ values of these magnitudes have historically been associated with the binding of cancer causing agents such as polycyclic aromatic hydrocarbons.
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Ionescu, Mihail  TM02, TO03
Iski, Erin  TM13, TP04
Jackson, Lauren  TP04
Jarshaw, Jane  TA05
Jaso, Vladislav  TM03
Javni, Ivan  TM03, TM04, GM01, GM02
Jimenez, Ashley  UM04
Jordan, Michael  TC02
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Kadel, Lava Raj  TR01
Kadossov, Evgueni B.  TE02
Kelsey, Jarred  TP01
Koshy, Jency  TC01
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Legler, C. R.  TP02
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The ACS MoKanOk Section would like to express our gratitude to Pittsburg State University and the Kansas Technology Center for the use of their facilities for the 60th ACS Pentasectional Meeting. We would also like to express our thanks to the Pittsburg State University Chemistry Club for their help.