

### Detailed Schedule

47<sup>th</sup> ACS DFW Meeting in Miniature  
Texas Wesleyan University, Fort Worth, Texas  
Saturday, April 26, 2014

7:45 – 8:30 AM Check-in (McFadden Science Center; Building 15)

8:30 – 9:45 AM Session 1

Physical/Inorganic 1 (Graduate)

Room: McFadden 102

**Kyralyssa Hauger**, Department of Chemistry, Texas Christian University  
*Synthesis and Characterization of Silylanilino Derivatives Containing Boron*

**Natalie Trinh**, Department of Chemistry, University of Texas at Dallas  
*Synthesis and Characterization of PIM-1/Cobalt SALEN as a Controlled and Site Specific NO Delivery Agent*

**J.P. Nimmo II**, Department of Chemistry and Biochemistry, The University of Texas at Arlington  
*First-principles studies of Amorphous Silicon Oxycarbide: Relating Structure to <sup>29</sup>Si NMR Data*

**Rebecca Weber**, Department of Chemistry, University of North Texas  
*The Effects of DFT Functionals on the Structures of Lanthanide Trifluorides*

Physical/Inorganic (Graduate)

Room: McFadden 304

**Eugenia Narh**, Department of Chemistry and Biochemistry, The University of Texas at Arlington  
*Structure-activity Relationships and Redox Activity of Bioreducible Ruthenium(II) Polypyridyl Complexes*

**Chris Jeffrey**, Department of Chemistry, University of North Texas  
*Gauging Performance of Density Functionals for Determination of the Structure of Lanthanide Trifluorides*

**Zainab H. Alsunaidi**, Department of Chemistry, University of North Texas  
*Amination of Benzene on the Ni (111) Surface: A Computational Study*

**Anne Marti**, Department of Chemistry, University of Texas at Dallas  
*The Fabrication of a Zeolite Imidazolate Framework (ZIF) Membrane for the Separation of Ethanol from Water*

Organic/Biochem/Polymer 1 (Undergraduate)

Room: McFadden 203

**Kevin J. Bruemmer**, Department of Chemistry, Southern Methodist University  
*<sup>19</sup>F Magnetic Resonance Oxidative Decarbonylation Reaction-based Probes for the Specific Detection of Peroxynitrite*

**Matt Sherman**, Department of Chemistry, Texas Christian University  
*Synthetic Caffeine Riboswitches as Genetic and Analytical Tools*

**Cindy Nguyen**, Department of Chemistry, University of Texas at Dallas  
*Use of Colloidal Metal-Organic Frameworks (MOFs) as Multifunctional Compatibilizers for Immiscible Polyimide/Polybenzimidazole Blend Membranes*

**Dalton Kim**, Department of Chemistry, Southern Methodist University  
*Modification of Polyphosphazenes by Copper-catalyzed Reactions*

9:45 – 10:00 AM Break

10:00 – 11:30 AM Session 2

Physical/Inorganic 3 (Graduate)

Room: McFadden 102

**Tejaswi Bhavanam**, Department of Chemistry, Texas A&M University–Commerce  
*Synthesis, Modification, and Characterization of Supported Gold Catalysts for Selective Hydrogenation of Acetylene in the Presence of Ethylene*

**Matthew J. Carlson**, Department of Chemistry, University of North Texas  
*Exploration of Weighted Core-valence Basis Sets for the Correlation Consistent Composite Approach for Transition Metals*

**Do Nguyen**, Department of Chemistry, University of Texas at Dallas  
*A Fast and Facile Synthetic Route for Zeolitic Imidazolate Framework 11 Nanoparticles*

**Dani Setiawan**, Department of Chemistry, Southern Methodist University  
*A New Approach for a Quantitative Description of Aromatic and Antiaromatic Molecules Based on Vibrational Spectroscopy*

Physical/Inorganic 4 (Graduate)

Room: McFadden 304

**Michael R. Jones**, Department of Chemistry, University of North Texas  
*Tyrosine-Phosphorylation in the Activity of Inhibitor of  $\kappa$ B Kinase- $\beta$*

**Jiaqi Wang**, Department of Chemistry, University of North Texas  
*Computational Study of the Oxidative Cleavage of C-H, C-C, C-O Bonds by Late First-Row and Second-Row Transition Metal Atoms*

**Alan Humason**, Department of Chemistry, Southern Methodist University  
*What is the Longest Carbon-Carbon Bond in Chemistry? Investigation of 11,11-Dimethyl-1,6-methano[10]annulene*

**Sajani A. Basnayake**, Department of Chemistry, University of Texas at Dallas  
*Synthesis of a Novel Metal Organic Framework (MOF) Using a Novel Linker*

**Zahra Bassampour**, Department of Chemistry, Southern Methodist University  
*Selective Nucleophilic Replacement Reactions of Substituted Silanes*

Organic/Biochem/Polymer 2 (Undergraduate)

Room: McFadden 203

**My-Linh Van**, Department of Chemistry, University of Texas at Dallas  
*Enzyme Immobilization in a Metal-Organic Framework*

**Margaret J. Risher**, Department of Chemistry, Tarleton State University  
*Isolation and Characterization of Isoflavones from Osage Orange L. Project-based Laboratory Exercises for Introductory Organic Chemistry*

**Daniel Galles**, Department of Chemistry, University of Texas at Dallas  
*Coated Acrylonitrile-based Terpolymer Prolongs Release of NO for Wound Healing Applications*

**Mai Khong**, Department of Chemistry, University of Texas at Dallas  
*Fabrication of Porous Carbon Nanofibers for Supercapacitors using Polybenzimidazole Incorporating Colloidal ZIF-8 Nanocrystals*

**Michael Tshisekedi**, Department of Chemistry and Biochemistry, Texas Wesleyan University  
*Synthesis and Evaluation of Novel DHFR Inhibitors*

11:30 – 1:00 PM Lunch (on your own)

1:00 – 2:30 PM

Session 3

Physical/Inorganic 5 (Graduate)

Room: McFadden 102

**Christopher South**, Department of Chemistry, University of North Texas  
*Analysis of the Electronic Structure of NdF<sup>+</sup> in Low Oxidation States*

**Imalka Munaweera**, Department of Chemistry, University of Texas at Dallas  
*Novel Chemoradiotherapeutic Magnetic Nanoparticles for the Targeted Treatment of Non-small Cell Lung Cancer*

**Atreyi Dasmahapatra**, Department of Chemistry and Biochemistry, The University of Texas at Arlington  
*Structure and Thermochemistry of Hafnia-Silica Glasses*

**Michele S. McAfee**, Department of Chemistry, Texas Christian University  
*Polymer Diffusiophoresis and Salt Osmotic Diffusion in Aqueous Salt Solutions*

Physical/Inorganic 6 (Graduate)

Room: McFadden 101

**Wijayantha A. Perera**, Department of Chemistry, University of Texas at Dallas  
*Sodium Niobate Nanorods and Nanotubes – Graphene Binder Free Nanocomposite Flexible Paper Electrode for Supercapacitors*

**Nathanael Mayo**, Nanotech Institute, University of Texas at Dallas  
*Flexible Transparent Loudspeakers*

**Blake Wilson**, Department of Chemistry, University of Texas at Dallas  
*Calculation of the Isothermal – Isobaric Partition Function using Nested Sampling*

**Andrew Mahler**, Department of Chemistry, University of North Texas  
*Correlation Consistent Basis Sets for In–Xe*

Physical/Inorganic 1 (Undergraduate)

Room: McFadden 304

**David M. Marolf**, Department of Chemistry, Abilene Christian University  
*New Triosmium Clusters with Multidentate Phosphine Ligands*

**Rawan Muhanna**, Department of Chemistry, University of Texas at Dallas  
*Synthesis of Novel Imidazole Linkers to Create Novel ZIF Structures*

**Minh Hoa Nguyen**, Department of Chemistry, University of Texas at Dallas  
*Transition Metal Complexes for Storage and Delivery of Nitric Oxide*

**Susana Aguirre-Medel**, Department of Chemistry and Biochemistry, The University of Texas at Arlington  
*Surface Functionalization of  $\beta$ -SiC Quantum Dots*

Physical/Inorganic 2(Undergraduate)

Room: McFadden 203

**Kenneth J. MacKenzie**, Department of Chemistry, University of Texas at Dallas  
*Adsorption of Nucleotides by bio-MOF-1*

**Zijun Yu**, Department of Chemistry, University of North Texas  
*Comparison of Density Functional Methods for Lanthanide Compounds*

**Prajay Patel**, Department of Chemistry and Biochemistry, The University of Texas at Arlington  
*Investigations of the Rhombohedral-to-cubic Transformation Path in Boron Nitride*

**Soo Hun Yoon**, Department of Chemistry, Abilene Christian University  
*Synthesis of Coordination Polymers Containing Diosmium Units*

Organic/Biochem/Polymer 1 (Graduate)

Room: McFadden 108

**Houliang Tang**, Department of Chemistry, Southern Methodist University  
*Synthesis and Functionalization of Disulfide-containing Polycyanoacrylates*

**Diego A. Lopez**, Department of Chemistry and Biochemistry, The University of Texas at Arlington  
*Vitamin B1 Pathway: A Distinct Source for Novel Antibacterial Development*

**Sara Merrikhihaghi**, Department of Chemistry, Southern Methodist University  
*Fluorescent Probes for Imaging Reactive Nitrogen and Sulfur Species*

**Nimali Abeykoon**, Department of Chemistry, University of Texas at Dallas  
*Supercapacitor Performance of Carbon Nanofibers Derived from PAN/PMMA Polymer Blends*

**Hongzhang Han**, Department of Chemistry, Southern Methodist University  
*Functional Polymer Materials with Complex Architectures Produced by Using Exchange Reactions at Hypervalent Iodine Center*

**Pradeep Budhathoki**, Department of Chemistry, Texas Christian University  
*Reversible Modification of the N-terminal Cysteine Residue of Proteins using Pyruvic Acid Analogs*

Organic/Biochem/Polymer 2 (Graduate)

Room: McFadden 306

**Jameela Lokhandwala**, Department of Chemistry, Southern Methodist University  
*Structural Characterization of Fungal Photoreceptor-Envoy*

**Jian Cao**, Department of Chemistry, Southern Methodist University  
*1,2-Dioxetane Chemiluminescent Probes for Imaging H<sub>2</sub>S in Living Cells*

**Rangana Jayawickramage**, Department of Chemistry, University of Texas at Dallas  
*Enhanced Conductivity of 1-Butyl-1-methylpyrrolidiniumbis(trifluoromethylsulfonyl)imide as an Electrolyte Double Layer Capacitor*

**Sahila Peranathan**, Department of Chemistry, University of Texas at Dallas  
*Supercapacitor Electrode Material from Immiscible Polymer Blends*

**David C. McLeod**, Department of Chemistry, Southern Methodist University  
*Controlled Radical Polymerization of 4-Vinylphenyloxirane to Produce Highly Functionalized, Well-defined Homopolymers and Block Copolymers of Various Architectures*

**Zhaoxu Wang**, Department of Chemistry, Southern Methodist University  
*Well-defined Redox-active and Fluorescent Polymer Prepared by Atom Transfer Radical Polymerization and Viologen-containing Initiator*

2:30 – 3:00 PM Break

3:00 – 4:00 PM Awards closing remarks (Bragan Fellowship Hall, ; Building 11)