## Conference Schedule

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<td>9:25-9:55</td>
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## Oral Presentation (Banquet Room B)

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<td>Dr. Ronald Tackett</td>
<td>Specialization and optimization of metal-oxide nanoparticles for use in the magnetic hyperthermia treatment of cancer</td>
<td>Kettering University</td>
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<td>2</td>
<td>Dr. Kai Trepte</td>
<td>Chemical bonding information from Fermi-orbital descriptors</td>
<td>CMU</td>
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<td>3</td>
<td>Dr. Martin Crimp</td>
<td>From Atoms to Autos: The Role of Crystallography in Deformation, Damage, and Fracture</td>
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<td>4</td>
<td>Dr. Jason Pagano</td>
<td>Metal salt crystals toward the synthesis of precipitation tubes</td>
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<td>Fatigue Behavior of Metal Alloys for Energy and Transportation</td>
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<td>7</td>
<td>Dr. Gabriel Caruntu</td>
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<td>8</td>
<td>Dr. Jerzy Klosin*</td>
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## Poster Presentation (Banquet Room A)

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<td>¹SVSU Great Lakes Bay Early College, ²Midland High School, ³Dow High School, ⁴Freeland High School, ⁵Michigan State University</td>
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Oral Session

Keynote Lecture
Dr. Jerzy Klosin, Dow

Title: “Development of Molecular Catalysts for the Production of Ethylene-Based Copolymers”

Abstract: The Dow Chemical Company is world's largest practitioner of homogenous catalysis including production of polyolefins. Olefin polymerization with homogeneous catalysts allows for unprecedented control over polymer composition and microstructure. This talk will discuss the development of new molecular catalysts within Dow for the production of ethylene-based copolymers such as ethylene-styrene and ethylene-1-octene. Particular emphasis will be giving to the recent research aimed at modifying structures of catalysts to affect both the polymer molecular weight and the reactivity toward alpha-olefins during ethylene/alpha-olefins copolymerization reactions.

Invited Lecture
Prof. Ronald Tackett, Kettering University

Title: “Specialization and optimization of metal-oxide nanoparticles for use in the magnetic hyperthermia treatment of cancer”

Abstract: The use of colloidal suspensions of ultrafine ferro(ferri-)magnetic materials (ferrofluids) in the magnetic fluid hyperthermia (MFH) treatment of malignant tumors has gained traction in recent years due to its non-invasive nature as compared to currently available treatments. This process, which involves exposure of the ferrofluid to alternating magnetic fields with amplitudes in the range from 0 – 15 kA/m and frequencies in the RF range, is dependent on many factors such as anisotropy, magnetic susceptibility, particle size, and the nature of the surfactant used. Much of the work done in this area centers around the use of superparamagnetic iron-oxide nanoparticles (SPION) due to their ease of synthesis and relative biocompatibility; however, due to the large Curie temperature (~580 °C) of these SPION a temperature feedback loop must be used during treatment to hold the malignant tissue at the requisite therapeutic time and temperature of 30 minutes at 42 °C. To combat this issue, we propose the use of silica-coated strontium-doped lanthanum manganite (La$_{1-x}$Sr$_x$MnO$_3$) which has a tunable Curie temperature (based on strontium content) in the desired therapeutic range. Using colloidal suspensions of these particles eliminates the need for this feedback loop as the temperature will oscillate around this Curie temperature as the materials repeatedly change from the ferro(ferr-)magnetic state to the paramagnetic state. In addition, preliminary investigations of the use of gadolinium-doping in an Fe$_3$O$_4$ system will be presented as a manner with which to increase the magnetic susceptibility, and thus rate of energy absorption, of the ferrofluids.

Invited Lecture
Prof. Martin Crimp, Michigan State University

Title: “From Atoms to Autos: The Role of Crystallography in Deformation, Damage, and Fracture”

Abstract: The vast majority of metals and a very large fraction of ceramics display long-range crystalline structures, with a broad variety of different structures developing depending on
composition and environmental conditions. Because of the directionality of the bonding in such crystals, the resulting properties, including thermal, electrical, optical, and mechanical, are typically anisotropic and can often be assessed in terms of the specific crystal structure. Such anisotropy is most dramatically evident in single crystals, and many applications reflect this, ranging from functional materials to high temperature turbine blades. Nevertheless, many engineering applications have historically ignored crystal anisotropy, as properties can often be “averaged out” if the individual crystals (grains) are randomly oriented in the polycrystal. In reality, however, polycrystals often have non-random crystal orientation distributions, known as crystallographic texture. Such textures can be developed in almost all processing schemes, including traditional processes, such as casting, rolling, extrusion, as well as more advanced processes such as sputtering, evaporation, and other thin film technologies. While the anisotropic behavior of materials can often be traced directly to their crystal structures, the nature of the boundaries between the grains can also play an important role in the final properties in polycrystals. In turn, properties of such grain boundaries will be controlled by not only the underlying crystal structures, but also the disorientation between the crystals on either side of a boundary and the orientation of the boundary itself.

At Michigan State University, we have considerable efforts focusing on the sources and manifestations of anisotropic materials behavior. Many, but not all, of these studies focus on the mechanical behavior of structural metals. A wide range of experimental approaches are used for studying these materials, including transmission electron microscopy (TEM), scanning electron microscopy (SEM), including in-situ deformation and heating experiments, and a variety of x-ray diffraction (XRD) approaches, including high flux beamline approaches. In particular, we have been at the forefront of development of techniques that allow high spatial resolution crystallographic studies using SEM to carry out studies historically limited to TEM approaches, including electron backscattered diffraction (EBSD) and electron channeling contrast imaging (ECCI). These approaches facilitate greater throughput and flexibility by eliminating the constraints typically associated with the thin foils requisite for TEM.

This talk will begin with a review of the general nature of crystalline materials and the properties that can be influenced by the specifics of the underlying crystallography. The experimental techniques that allow the crystallographically influenced behavior of the materials to be understood at a mechanistic level will be discussed. Following this, a number of examples of anisotropic structure-property relationship studies will be presented. Particular focus will be given to mechanical behavior studies that are mechanistically controlled by the nature of dislocation structures and motion, including how the interaction of these crystal defects with the boundaries between grains influences the deformation and fracture behavior of structural materials.

**Invited Lecture**

**Prof. J. Wayne Jones, University of Michigan**

**Title:** “From Defects to Microstructure Neighborhoods: Fatigue Behavior of Metal Alloys for Energy and Transportation”

**Abstract:** Fatigue failure is often the life limiting characteristic of structural alloys and the possibility of fatigue failure limits both the stresses that components can support and the safe service life of critical components. In aerospace, automotive and energy production rotating components are critical, and their failure would be catastrophic. Under many circumstances fatigue lifetimes may reach $10^6$-$10^{10}$ cycles and predicting when failures will occur and designing to prevent them are becoming increasingly important. In this very high cycle fatigue (VHCF) regime fatigue lifetime is controlled by fatigue crack initiation and, in some cases, small fatigue
crack growth behavior. A fundamental aspect of this behavior is that a hierarchy of microstructure features can be identified that directly influences fatigue life through their influence on initiation and small fatigue crack growth behavior. In many commercial alloys features such as porosity or inclusions are critical. In other advanced alloys where such features are minimized microstructural variability and the characteristics of specific microstructural neighborhoods become the dominant influence on fatigue life. This presentation briefly provides a background of the fundamentals of fatigue and then reviews research over the past 20 years at the University of Michigan that has used ultrasonic fatigue methodologies to investigate the influence of microstructure on fatigue behavior in the VHCF regime for a wide range of structural alloys. Alloys examined using ultrasonic fatigue include cast aluminum alloys, wrought magnesium alloys, titanium alloys and nickel base superalloys. Emphasis will be placed on how the research findings from this broad range of alloys can inform alloy design and fatigue life prediction.

**Invited Lecture**

**Prof. Gabriel Caruntu, Central Michigan University**

**Title:** “Solution-Processed Ferroelectric Perovskite Colloidal Nanocrystals for Flexible Electronics”

**Abstract:** Ferroelectric perovskites are among the most technologically important inorganic materials which have been used in many cutting-edge technologies, ranging from cellular imaging, to energy conversion and storage, catalysis, electrocaloric refrigeration, piezoelectric devices, electronics and high density data storage. Despite the enormous technological potential of low-dimensional perovskites, the current knowledge on their proprieties is far less advanced than that on single crystalline and bulk materials. We describe in this talk the structure of the nanoscale polarization and the scaling limit of the polar ordering in high quality, aggregate-free, monodisperse colloidal nanocrystals of BaTiO₃, an archetypal ferroelectric perovskite. Fine chemical synthesis in tandem with selective solvent evaporation techniques enable the manipulation and isolation of individual nanoparticles allowing the examination of the local structural and electrical behavior in individual nanocrystals with an unprecedented resolution. In-situ electron microscopy revealed that ferroelectricity persists down to 5 nm in BaTiO₃ nanoparticles with the retention of a primarily linear, monodomain dielectric polarization. These findings provide for the first time a glimpse into the structural and electrical manifestation of the polar ordering down to its ultimate size limits and can potentially result in the improvement of the actual design technologies in smart materials with programmable ferroelectric, dielectric and piezoelectric properties. In the last part of the talk, we describe our successful attempts to use BaTiO₃ colloidal nanoparticles as building blocks to fabricate dielectric nanocrystal solids and integrate them into flexible electronics, such as capacitors and field-effect transistors, whose performance characteristics will be discussed in detail.

**Oral Presenter**

**Dr. Kai Trepte, Central Michigan University**

**Title:** “Chemical Bonding Information from Fermi-Orbital Descriptors”

**Abstract:** Calculations with density functional theory (DFT) provide accurate results at a low computational cost. However, most exchange-correlation functionals do not cancel the so-called self-interaction error, meaning that electrons artificially interact with themselves. To combat this, self-interaction corrections (SIC) have become important. One method is the Fermi-Löwdin orbital self-interaction correction (FLO-SIC). In this method, one needs to optimize points in space, the Fermi-orbital descriptors (FODs), to find the energy of the SIC energy functional for a given
system. We present an interpretation of FODs and argue that these descriptors carry chemical bonding information. We show that a bond order derived from these FODs agrees well with reference values and highlight that optimized FOD positions correspond to expectations from Linnett's double-quartet theory, which is an extension of Lewis theory.

**Oral Presenter**

Prof. Jason Pagano, Saginaw Valley State University

**Title:** “Metal Salt Crystals Toward the Synthesis of Precipitation Tubes”

**Abstract:** A “chemical garden” or “silica garden” may be described by crystals of metal salts which grow in an aqueous solution of sodium silicate (also known as waterglass). They are visually pleasing and resemble the forms of a garden. Demonstrations of this experiment are well-known, and different tube colors and shapes can form depending on the type of metal salt used. Using this “chemical garden” or “silica garden” reaction-precipitation system, we investigate the growth dynamics of hollow precipitation tubes formed from reactant-loaded seed crystals. The latter crystals form by sedimentation from a mixture of aqueous solutions containing alum and copper(II) sulfate. During the experiment, a single crystal (100 to 1000 mg in mass) is placed in a small volume of sodium silicate (V = 25-30 mL) such that the formation of precipitation structures is monitored by a time-lapse camera. All experiments are conducted at ambient temperature (T = 23±1 °C). At low concentrations of sodium silicate (1.0 M), the tube growth is characteristic of the budding regime. For high concentrations of sodium silicate (6.25 M), tubes are initially directed by a single gas bubble. Over time, the structures expand and form chemical balloons at the column base of the aluminum/copper/silica precipitation structure. Using an experimental methodology consisting of both image acquisition and processing we are able to quantify the spatial and temporal dynamics. Systematic measurements include but are not limited to: tube radius, induction period, and growth velocity. Depending on the experimental conditions the volume of the structure may be calculated using two distinct mathematical techniques. The first technique is by geometry and integral calculus is the second. This presentation will also discuss both the qualitative and quantitative aspects of the distinct morphologies of precipitation tubes at reactive interfaces. Lastly, results from scanning electron microscopy and infrared spectroscopy will be presented.

**Oral Presenter**

Kalyn Froeschle, Dow

**Title:** “High Viscosity Mixing in a Cuboidal Tank”

**Abstract:** Mixing studies were conducted to understand a production mixing process where high viscosity fluids are mixed in a cuboidal portable tank with a cross-section of 42” x 48”. The goal was to validate whether the current tank and impeller design provide adequate mixing. The potential for stagnant material in the cube corners made it necessary to run lab-scale experiments. The blending was studied in a scaled-down cuboidal aquarium with nominal 9” sides. The model system used 500 cS fluid for two thirds of the volume and 55,000 cS fluid for the remaining third; ultramarine blue-pigment was mixed into the fluids to provide a qualitative and semi-quantitative assessment of homogeneity. Tests were run at several impeller sizes, tip speeds, and power/volume to quantify bulk mixing and ability to reduce stagnant material in the cube corners. A calibration curve was developed to measure dye concentration from spectrophotometer transmittance using Beer’s law to complement the qualitative dye motion observations with quantitative concentration measurement.
Initially, poor batch uniformity was expected due to the small D/T at the relatively high final viscosity of 5,000 cP (D/T = 0.3 imposed rather than a preferred D/T = 0.5). However, mixing experiments revealed that the critical requirement to ensure batch uniformity is to have an impeller Reynolds number high enough in the transitional regime (Re~200) to avoid stagnant regions in the four lower cube corners (Re<80), which are the last region to mix in this geometry. Appropriate calculations confirmed that the production tote mixer can generate the required Reynolds numbers when running the tote mixer setup at the full speed and that the mixer itself has the power required in this system.
1. Catalysis of a Polymerization Using Polymer Chain Folding and Macromolecular Structure

Ryan Baumgartner, Dow

Catalysis observed in enzymatic processes and protein-based polymerizations often relies on the use of supramolecular interactions and the organization of functional elements in order to gain control over the spatial and temporal elements of fundamental cellular processes. For example, tubulin polymerization is aided by microtubule-organizing centers such as the centrosome. The polymerization of actin is similarly stimulated by the Arp2/3 complex. These nucleation factors catalyze polymer growth by lowering the activation energy of nucleation while also regulating the organization of the resulting polymeric arrays. At present, there are few man-made polymerization systems that are able to harness the supramolecular interactions that nature uses to catalyze and direct the growth of polymers. Here, a fundamentally new polymerization system is developed that utilizes the macromolecular structure of the polymer as a catalyst for its own growth. We show that not only does the formation of α-helices act to catalyze a polymerization, but the organization of the α-helices in the macromolecular architecture can increase the polymerization rate by over 1000-fold. The system consists of a linear polymeric scaffold containing initiation sites on which amino acid precursors, in the form of N-carboxyanhydrides (NCAs), condense to form polypeptide chains. Upon reaching a critical chain length, the polypeptide chains are able to fold into α-helices. The continued addition of NCA monomers onto the α-helices is found to be catalyzed through cooperative dipolar interactions between neighboring α-helices on the same scaffold. By controlling the structural elements that govern the proximity of growing helices along the scaffold, the extent of this effect on the polymerization can be modulated. This represents the first known example of a cooperative polymerization that forms covalent bonds.

2. Measuring the Antibacterial Efficacy of Essential Oils on Staphylococcus epidermidis

Miaela Gisch & Joshua Lang, SVSU

Staphylococcus epidermidis readily colonizes on human epithelia. Despite its seemingly benign nature, it is an opportunistic pathogen, and can prove difficult to eradicate upon infection. It is thus important to identify effective antibacterial agents for S. epidermidis. The aim of this study was to qualitatively and quantitatively assess the S. epidermidis antibacterial efficacy of lavender, lemongrass, cinnamon, and clove essential oils. Antibacterial activity was assessed qualitatively by inhibition of bacterial growth using a Kirby-Bauer disk diffusion assay, along with household diffusers and household hand sprayers applied to tryptic soy agar plates cultured with S. epidermidis. Antibacterial activity was assessed qualitatively by inhibition of bacterial growth using a Kirby-Bauer disk diffusion assay, along with household diffusers and household hand sprayers applied to tryptic soy agar plates cultured with S. epidermidis. Antibacterial activity was assessed qualitatively by inhibition of bacterial growth using a Kirby-Bauer disk diffusion assay, along with household diffusers and household hand sprayers applied to tryptic soy agar plates cultured with S. epidermidis. Concentrations of active ingredients were determined quantitatively using an internal standard calibration method with a gas chromatograph mass spectrometer (GCMS). This method was used in conjunction with the Kirby-Bauer disk diffusion assays to determine the minimum inhibitory concentrations of active ingredients in the essential oils required for inhibition of S. epidermidis growth on tryptic soy agar plates. Lemongrass, cinnamon, and clove oil all showed effectiveness at inhibiting the growth of S. epidermidis using the disk diffusion assay, while
lavender oil did not; however, preliminary results show that diffusers and hand sprayers containing clove and lemongrass essential oils are ineffective at inhibiting S. epidermidis growth.

3. Towards More Stable and Ion-Conductive Organic Electrolytes for Rechargeable Lithium-Oxygen Batteries

Shuting Feng, Dow

The global society urgently needs to remedy the effects of climate change and increase the utilization of renewable energy. Rechargeable batteries are important enablers of sustainable energy use, as they can be employed to store energy generated from renewable but intermittent source. Enhancing the functionality of battery electrolytes can improve battery energy density, operation efficiency, and safety. This poster discusses strategies to improve the stability and ion conductivity of organic electrolytes for rechargeable batteries. Special attention is given to aprotic lithium-oxygen (Li-O$_2$) batteries, which offer theoretical energy densities that are 2 to 4 times increase over the state-of-the-art Li-ion batteries (LIBs). Currently, the practical development of rechargeable Li-O$_2$ batteries is hindered by severe electrolyte degradations. Numerous families of organic solvents, polymers, and ionic liquids have been evaluated as electrolyte candidates; none are stable against the oxygen electrode in Li-O$_2$ batteries. Moreover, the decomposition pathways of many molecules are poorly understood. To investigate the structure-property relationships governing the stability of organic molecules in aprotic Li-O$_2$ electrode environment, we developed and applied a comprehensive stability framework to a library of organic molecules with varied functionalities using density functional theory (DFT) calculations. Additionally, the chemical stability of the molecules was investigated experimentally. The computed and experimental results were in excellent agreement and have been employed to identify unstable chemical moieties and to provide insight into the design of new electrolytes that would be stable in Li-O$_2$ battery environment. Using the guiding principles provided by this stability framework, we developed three sulfamide- and sulfonamide- based electrolyte solvents that exhibited exceptional stability under aprotic Li-O$_2$ conditions. In particular, the sulfonamide-based electrolytes have been found to be stable for >90 cycles in a Li-O$_2$ cell, highlighting the power of rational molecular design for the development of stable and ion-conductive organic electrolytes for next-generation batteries.

4. Progress Towards an $^{19}$F Magnetic Resonance Probe for Monitoring Acetylcholinesterase Activity

Kyle Minder, UM-Flint

Acetylcholinesterase (AChE) activity is largely responsible for terminating neurotransmission associated with acetylcholine. Under normal conditions, AChE hydrolyzes receptor-bound acetylcholine on the post-synaptic membrane. Alzheimer’s and other central nervous system diseases, however, are characterized by premature termination of neurotransmission owing to AChE activity. Thus, the ability to monitor changes in AChE activity may provide insight into the chemical mechanisms associated with neurodegenerative diseases. Recently, a fluorescent probe incorporating a dimethylcarbamate was shown to selectively respond to AChE activity given an increase in fluorescent response following hydrolysis of the target dimethylcarbamate. This approach, however, is limited to in vitro imaging applications given the poor penetration depth of visible light. To address this issue, we report progress towards an $^{19}$F magnetic resonance (MR) probe capable of responding to AChE activity. Hydrolysis of a dimethylcarbamate to the corresponding phenol is expected to initiate a self-immolative cascade and concomitant shift in the $^{19}$F MR response. This approach has been applied previously within our group to elicit a chemoselective response in the presence of the reactive oxygen species H$_2$O$_2$. 
5. Fermi-Löwdin Orbital Self-Interaction Correction Theory applied on Small Water Clusters

Kamal Sharkas, CMU

Kohn-Sham density-functional theory (KS-DFT) is a very important computational method of modern quantum chemistry with applications ranging from small molecular systems to solid state. Though DFT reaches chemical accuracy for many applications, self-interaction error (SIE) remains a one of the still unresolved problems in present-day functionals. The Fermi-Löwdin Orbital Self-Interaction Correction (FLO-SIC) \[1\] methodology was recently introduced as a proper variational reformulation of the Perdew-Zunger SIC scheme \[2\].

After a brief review of the theory, we present the application of FLO-SIC on small water clusters by assessing their binding energies against benchmark values. In particular, we show that FLOSIC-SCAN performs better than the SCAN functional by yielding improved binding energies and preserving their correct ordering for the prism, cage, book, and ring isomers of water hexamer.

6. Air Barriers and Water Vapor Permeation in the High Performance Building Market

Milton Repollet Pedrosa, Dow

Over the last decade, the air barrier market has grown with a broad range of technology offerings including urethane-, silicone-, and acrylic-based systems. In 2013, Dow Performance Silicones started the Build a Better Barrier Program to introduce unique silicone technologies to the air barrier market. As the air barrier market grew, more and more architects, contractors, and consultants were asking Dow Performance Silicones for water vapor permeance values. The advancement of technologies in this space, whether permeable, semi-permeable and impermeable, have created a debate on how permeability of an air barrier matters and how buildings benefit from it. This presentation will discuss the study of the water vapor transmission rate and permeance of commercially available air barrier technologies at specified sets of temperature and humidity. We will describe the current landscape of technologies and their water vapor transmission rates emphasizing an accurate comparison between different air barriers to compare performance attributes. We will discuss how this information enables our understanding on how to build better air barrier systems that benefit the building envelop and, ultimately, its durability.

7. 28 Years of Exceptional and Significant Contributions of the Mid-Michigan Technician Group

Kyle Krauseneck, Dow

For the past twenty eight years, the Mid-Michigan Technician Group has been focused on promoting personal and career related growth throughout the Technician community. Current and past members have participated in numerous public outreach events such as Kids and Chemistry, Sci Fest, ACS Day at the Fair, and many more. MMTG has sponsored or volunteered it’s time to both the science community and those interested in working in a science related field. MMTG and their members have received various awards from their contribution to the community and the promotion of technicians.

8. Mechanical Reliability of Novel 3D-Printed ABS-Graphene Composites

Peter Kozerski, H.H. Dow High School
3D printing is one of the fastest-growing segments for manufacturing and production. This success is attributed to the increased use of 3D printing not only for rapid prototyping but also final models and production parts. The reliability of plastic parts is a critical factor in their engineering applications. Previous research pursued on novel nanocomposites based upon Acrylonitrile Butadiene Styrene (ABS) compounded with XGnP™ graphene nanoplatelets at the 5 wt. % and 10 wt. % levels indicated that stiffness doubled, and toughness decreased by a factor of 4 over the 10 wt.% content range. In this study, test samples were fabricated from these novel ABS blends and characterized for their mechanical properties using tensile testing. 3D printed ASTM tensile samples, which had a defined 3 mm diameter circular hole geometry in the center, were characterized to determine their influence on the mechanical properties and reliability. Both material and 3D printing fabrication variables were being assessed. The reliability of the mechanical properties of specimens was estimated with the use of Weibull statistical analysis to determine the probability of failure. Results supported the previous relation between elastic modulus and graphene addition with approximately double elastic modulus over 10 wt. % graphene content. However, the 10 wt. % graphene addition lowered or maintained the same yield stresses compared to 0 wt. %, possibly due to the presence of the hole and potential associated defects in specimens. Weibull analyses indicated the 10 wt. % addition decreased Weibull modulus by 2/3, which increased the broadness of failure. The introduction of a hole decreased yield stress yet increased Weibull modulus. This study provided an understanding of how to achieve the desired reliability levels for 3D printed parts made from the novel ABS nanocomposites.

9. Fabrication of Biomaterials for Bone Repair and Regeneration

Grace Bremmer, H.H. Dow High School

3D printing technology has been widely used in the fabrication of biomaterials for tissue engineering. There would be value in determining the degree to which one may fashion scaffolds with readily available low-cost polymer filaments using affordable 3D printers, particularly for early-stage prototyping. This research focused on the bone defect area of tissue engineering. Bone defects, both congenital and acquired, are serious and costly impairments. Beyond a critical size the defects (i.e., fractures) are not able to heal without further medical intervention. An effective treatment technique is to implant a biodegradable scaffold at the injured site to promote bone regeneration by attracting cells to the area. Using additive manufacturing, scaffolds can be fabricated to the specific needs of patients. In this study, scaffolds were modeled and fabricated in the form of a cube using various polymers and biopolymers (e.g., PCL, PLA, PVA, PLA/PHA, and an olefin block copolymer) with different geometric configurations and infill percentages. The mechanical properties of the scaffolds were characterized using compression tests to determine the yield stresses and compressive Young’s moduli. The reliability of the mechanical properties of scaffolds was estimated with the use of Weibull statistical analysis to determine a probability of failure. The results were compared with yield stresses and moduli of different trabecular bone tissues at multiple anatomical locations, and enhanced understanding of the structural optimization of polymer scaffolds and as an aid to tissue regeneration for bone defects.

10. Synthesis, Microscopy and Spectroscopic Characterizations of Rare Earth- Doped BaTiO₃ Nanocubes for Optical and Feroelectric Applications

Benard Kavey, CMU

Rare-earth doped BaTiO₃ nanocubes have been synthesized using a highly versatile, energy-efficient solvothermal route at temperatures as low as 150 °C. Transmission electron microscopy
images of the as-synthesized Ba$_{1-x}$Ln$_x$TiO$_3$ (0.01≤ x ≤0.09; Ln = La$^{3+}$, Ce$^{3+}$, Nd$^{3+}$) showed highly monodisperse and self-assembled nanocubes with a mean particle size of 20 ± 2 nm for all nominal dopant compositions. High resolution transmission electron microscopy was used to explore in detail the atomic planes, polarization direction, distribution of individual dipoles and the ferroelectric domains within a single nanocube. Also, piezoelectric force microscopy and lithography techniques were employed to further understand the ferroelectric behavior of the Ba$_{1-x}$Ln$_x$TiO$_3$ nanocubes. It was determined that all Ba$_{1-x}$Ln$_x$TiO$_3$ nanocrystals present a ferroelectric behavior at room temperature with maximum values of the permittivity around the Curie temperature. Dielectric spectroscopy measurements were performed by using vacuum sintered pellets of the as-synthesized nanocubes and measured at both the megahertz and terahertz electric field frequencies. We observed significantly higher dielectric constant values up to 6000 for lower Ln$^{3+}$ dopant concentrations. An FTIR technique was employed to study the surface characteristics of the nanocubes and the nature of binding of the capping ligand molecules to the surface of the nanocrystals. It was determined that the oleic acid ligand used as a capping agent binds to the Ba$^{2+}$ ions in the Ba$_{1-x}$Ln$_x$TiO$_3$ crystal structure via a bidentate coordination mechanism. The insulating properties of the Ba$_{1-x}$Ln$_x$TiO$_3$ was further determined using diffuse reflectance spectroscopy and the Kubelka-Munk theory of reflectance. The band gaps of the as-synthesized Ba$_{1-x}$Ln$_x$TiO$_3$ nanocubes were determined for all different Ln$^{3+}$ dopants and various concentrations.

11. Ocean Trash to Ocean Treasure

*Isaac Hales, Valley Lutheran High School*

I decided that I wanted to look at plastic waste in the ocean and what could be done with it. Cement is the 2nd most consumed material besides water. Plastic waste in the ocean is compounding at a rate of 8 million tons per year. Taking recycled plastic I treated the plastic with silane compounds and mixed with water, then I put the nylon fibers in a silane solution and then in the cement. I was able to create a substance that would help the plastic fibers adhere to the cement compound. I was able to create cement that was lighter and strong than without the plastic fibers. This combination of recycled plastic that is treated with a silane solution and cement could help reduce plastic waste in the ocean and create better and stronger cement for industry. This will help save the oceans from pollution while reducing cement costs.

12. Modeling of Silicone Rubber in Sigma Blade Mixers

*Andy Kenney, Dow*

Computational fluid dynamics (CFD) modeling has enabled a deeper understanding of complex mixing of high viscosity materials that enables more predictable decisions when designing process equipment. In industry, this translates to more effective investments that target improved efficiency and productivity as a result of more informed design decisions. In silicone rubber, heating and cooling of the rubber is a mostly non-value added step within the production process that has a significant impact on cycle time and overall production capacity. In this instance, CFD modeling was used to model the heating and cooling of high viscosity uncured silicone rubber at different scales in sigma blade-style high viscosity mixers. This modeling was able to determine not only optimum heating and cooling conditions, but also enabled decision making on what mixer sizing would prove optimal for processing of similar material.

13. One Hundred Years of Midland Section ACS Chairpersons (1919-2019)
The Midland Section of the American Chemical Society has been an outstanding local section for one hundred years because of a large group of talented individual members and support from industrial and academic institutions within the Section. One important group of 91 individuals are the past and present members who have served as Section Chairpersons. All the members of this group are listed in this poster, starting with Herbert H. Dow in 1919 and ending with Amanda M. Palumbo in 2019. Most Section Chairpersons served for one year; the following served for more than one year: Herbert H. Dow, Thomas Griswold, Jr., Edgar C. Britton, Lawrence F. Martin, Laurence L. Ryden, David C. Young, Bob A. Howell, Thomas H. Lane, George W. Eastland, Jr., Gretchen S. Kohl, J. Patrick Cannady, and Regina M. Malczewski. These Section Chairpersons in consultation with the other officers set the goals and overall direction of the Section for the year. Several activities of the Section carried over for many years so the chair had the responsibility for ensuring these activities continued successfully, by delegating responsibilities, and recruiting and guiding new officers and committee chairpersons. For example, the Fall Scientific Meeting has continued for 75 years (1945-2019). The Chairperson of the Section served as the Chairperson of the Board of Directors and the Executive Committee, presided over their meetings, and appointed all committees authorized by the bylaws or by the Board of Directors, except the Chairperson and members of the Committee on Nominations and Elections. The Chairperson was responsible for the overall operation of the Section, presided over general meetings of the Section, and helped prepare the annual Section report. The authors of this poster have all served as Midland Section Chairpersons, DCY 1956-1957, REK 1994, WLD 2000, AMP 2019.

14. History of the Midland Section ACS Fall Scientific Meeting, 1945-2019, 75th Anniversary – General Chairs and Keynote Speakers

Wendell Dilling, CMU

The 2019 ACS Fall Scientific Meeting (FSM) is the 75th meeting of the series, which started in 1945. Early scientific meetings were organized by scientists at The Dow Chemical Company and Dow Corning Corporation and were attended mainly by employees of those companies. More recent FSM’s have been organized and attended by other scientists, academic scientists and students in addition to Dow and Dow Corning scientists. This poster traces some of the history of these meetings and lists all the dates, locations, and general chairs, starting with K. D. Gordon Clack in 1945 up to Elizabeth Santos and Tom Bekemeier in 2019. Also listed are the keynote speakers and their address titles of all the meetings starting with J. J. Grebe, “A Yardstick for a Ten Year Research Program” in 1955 up to Jerzy Klosin, “Development of Molecular Catalysts for the Production of Ethylene-Based Copolymers” in 2019. Three Nobel Prize winners and eleven ACS presidents have presented keynote addresses. Attendance figures will be presented in relation to the day of the week the FSM was held and other factors affecting attendance. Some other aspects of FSM’s will be reviewed: institution of poster papers in 1977, presentation of posters by Project SEED students starting in 1978, evolution of printed programs over the years, exhibits starting with the very first meeting in 1945, addition of chemical “magic shows” in 1987 and Sci-Fest programs in 1993. The financial assistance of The Dow Chemical Company and Dow Corning Corporation is gratefully acknowledged.

15. Philatelic Cachets from Central Reginal ACS Meetings Hosted by the Midland Section

Wendell Dilling, CMU
In philately, a cachet is a printed or stamped design or inscription, other than a cancellation or pre-printed postage, on an envelope or postcard to commemorate a postal or philatelic event. A first day cover is a stamp on an envelope postmarked on the first day of issue. Philatelic cachets have been issued at three of the Central Regional ACS Meetings hosted by the Midland Section, in 1997 in Midland, in 2006 in Frankenmuth, and in 2019 in Midland. The 1997 cachets commemorated the Chemis-Tree during National Chemistry Week and bringing science to life in the classroom, the Dow brine well as a historical chemical landmark, the 10th anniversary celebration of National Chemistry Week, and 100 years of Dow Chemical, 1897-1997. The 2006 cachets commemorated education and Jean-Michel Cousteau, the 2006 World Expo of Beer, and the 39th Silicon Symposium. The 2019 cachets celebrate the century of science and service by the Midland Section by featuring the discovery of Silly Putty by Earl Warrick in 1947, the discovery of Styrofoam by O. Ray McIntire in 1948, the discovery of Saran by Ralph Wiley in 1949, and the discovery of superabsorbent polymer by Frederic L. Buchholz in 1972.

16. Electrochemical Investigation of Ruthenium Complexes Utilizing Cyclic Voltammetry

Vincent Flores, SVSU

The complexes benzylidene-bis(tricyclohexylphosphine)-dichlororuthenium, and [1,3-bis-(2,4,6-trimethylphenyl)-2-imidazolidinylidene]dichlorophenylmethylene)tricyclohexylphosphine)ruthenium are well-known and extensively studied complexes. They are known for the wide range of reactions that they can be involved in. An area of interest that lacks in current literature is the redox properties of these complexes and their analogues. Our focus is to expand the knowledge of these complexes, more specifically, with respect to their first oxidation potential. Our group set out to investigate the electrochemical and spectroelectrochemical properties of these complexes as well as their analogues. The redox properties of these complexes have been examined utilizing cyclic voltammetry (CV) techniques using various solvents and electrolytes. The two different supporting electrolytes used in the CV experiments are tetrabutylammonium hexafluorophosphate and tetrabutylammonium tetrakis[3,5-bis(perfluorohexyl)phenyl]borate. The extensive CV experimentation includes the utilization of screen printed platinum and glassy carbon disk electrodes, as well as varying temperatures.

17. Synthesis and Electrochemistry of Rhodium Catalyst Analogues

Hayler Lillo, SVSU

Rhodium (I) based catalysts are used actively in industry as they efficiently hydrogenate unsaturated compounds. These types of organometallic catalysts are well-known and studied compounds, however, little research has been done regarding their electrochemical properties and that of their analogues. The primary goal of this project is to synthesize a number of rhodium (I) analogues by altering the substituents on the attached phenyl rings. Preparations of the analogues are practiced utilizing Schlenk-line (air- and moisture-free) techniques. Following synthesis, the compounds were checked for purity and extent of reaction completion using infrared (IR) spectroscopy and nuclear magnetic resonance (NMR). The electrochemical technique of cyclic voltammetry (CV) was used to find the substances’ oxidation and reduction potentials. The potentials of the analogues differed based on the given substituent attached to the phenyl rings. Spectroelectrochemical experiments were also used to assess structural changes upon oxidation.
18. Synthesis and Characterization of Ruthenium Metal Hydroxamate Complexes

Alice Erman, SVSU

In the field of chemistry, the interactions between biological compounds, such as the heme unit, and nitric oxide (NO) are thoroughly studied and researched. However, there is much more to be learned from molecules that have the ability to generate NO within a biological system. The goal of this project is to study the interactions between molecules that donate nitric oxide, and synthetic ruthenium-metal based models of the heme unit. In this study, hydroxamic acids are used as NO donating compounds. The focus of this research is to understand the redox behavior of the interactions between these compounds through the use of electrochemical and spectroelectrochemical techniques.

19. Higgins Lake Watershed Study: A Community-School Based Surface Water Monitoring Program

Chuck Schepke, Roscommon High School

This program utilizes high school chemistry students to sample, test and evaluate the Higgins Lake Watershed and tributaries in Michigan. Students would sample water from a number of sites within the land watershed and test for inorganics, bacteria and physical characteristics of the test site. Sampling has increased to 12 different sites within the watershed and has been performed each month during 2018. The first year of testing at each site is to obtain a base line of each test site for continued testing over the next five years. Each site database has been combined together to provide a complete, systematic picture of the quality of water in this important water shed over an extended period of time. Water analysis included a variety of EPA certified chemical analysis techniques. The water testing is performed and compared with EPA certified standards to ensure accurate, reliable test results. Using EPA standards reinforces the importance of using standards to compare testing technique, procedures and analyst ensuring quality data collection. This reinforces and connects the academic realm to real world job potentials. This is also part of a job-shadowing program within the watershed program to expose the students to potential employment opportunities available to qualified trained individuals.

20. Effects of Hygrothermal Conditions and Thixotropy on the Modulus Build of Moisture-Cure Silicone Sealants

Chrissy Marchand & Glenn Gordon, Dow

The kinetics of 1-part moisture-cure materials were described by Comyn and collaborators by assuming a diffusion-controlled mechanism where a cured layer advances from the surface inwards into the bulk of the material with a sharp boundary that depends on the permeability of moisture, the concentration of reactive sites, and water vapor pressure that functions as the driving force. It was subsequently demonstrated that the depth of cure into the bulk at different temperatures and humidities collapses into a single straight line when plotted versus the square root of the product of time and vapor pressure. Aside from asking how fast 1-part materials cure, customers also want to know the rates of mechanical and adhesion strength development. The
objective is to show the buildup of mechanical strength represented by the dynamic modulus of silicone sealants at different cure conditions also collapses into a single master curve unless the material is thixotropic.

21. Synthesis of C-Glycosides as Potential Treatment for Type II Diabetes

Rachel Laskowski, SVSU

Type II diabetes mellitus is a significant health problem worldwide and is largely characterized by hyperglycemia, which can lead to a variety of other diseases. Lifestyle changes can make the disease more manageable, but most patients also require drug therapy to fully manage hyperglycemia. Alpha-glucosidase inhibitors and sodium-glucose co-transporter 2 (SGLT2) inhibitors have both been used to reduce blood glucose levels. O-glycosides and C-glycosides have been used for this purpose. While O-glycosides tend to suffer from metabolic instability, C-glycosides are less prone to degradation and have the potential to be effective and selective SGLT2 inhibitors. This research project focuses on the synthesis of C-glycosides as potential compounds for treatment of type II diabetes. It is hypothesized that these compounds could potentially function as both alpha-glucosidase inhibitors and SGLT2 inhibitors. Three different synthetic pathways are currently being explored to prepare a variety of C-glycosides. The products of these reactions are purified using column chromatography and recrystallization. Analysis of spectra obtained through Nuclear Magnetic Resonance spectroscopy is used to ensure that the intended product is synthesized. This presentation will discuss the synthesis of the target C-glycosides.

22. Low Temperature Cure LSR Technology Enables Processing Improvements

Michael Wang, Dow

Liquid silicone rubber (LSR) has emerged as a preferred elastomeric material due to a combination of ease of processing and physical properties. These materials are generated by a platinum-catalyzed hydrosilylation reaction, which vulcanizes silicone polymers. Traditional processing conditions utilize liquid injection molding at high temperatures, typically 170-220 °C, to produce complex articles while allowing short cycle time and parts consistency. The introduction of a novel Low Temperature Cure (LTC) technology can greatly expand the benefits of LSR products. This new class of LSR allows for fast curing speeds at temperatures as low as 100 °C, enabling both optimized processing as well as new innovative process and product designs. Analysis of the cure performance of LTC technology demonstrates clear processing improvements in consumer, electronic, and automotive applications. At higher temperatures, LTC technology affords improved cycle times and fast deep-section cure (greater than 5 mm thickness). The performance of deep-section cure was evaluated using mold temperature simulations and was confirmed by a series of injection molding process studies.

At lower temperatures, the ability to vulcanize LTC LSR in the 100-120 °C range provides design flexibility and maximum process efficiency to the LSR portfolio. In addition to more efficient energy usage and heating times, this technology also enables comolding of LSR with low-melting
plastics, opening new markets for silicone molding. Another benefit is the option to add a cure accelerator to the LTC LSR which can further reduce the processing temperature to 90 °C, greatly enhance cycle time reduction, and speed up deep-section cure, all while maintaining physical properties and pot life. Low Temperature Cure LSR is an exciting new development that exhibits unparalleled performance throughout a broad processing range and excels at temperature ranging 90-120 °C. This new class of materials leverages platinum catalysis to drive consumer applications.

23. Effects of Alkyl Chain Length and Carbohydrate Stereochemistry on Gel Formation and Phosphate Removal

*Kathryn Richmond, SVSU*

Our laboratory is examining the synthesis of carbohydrate gelators. Previous work has explored how gel formation is affected by modifying the length of the nonpolar group attached to β-D-galactose. This project will attempt to continue this research by testing the effect of stereochemistry of the carbohydrate on gel formation by comparing gels formed with galactose to those formed with glucose. As well as that, we are continuing to determine the optimum chain length of the nonpolar group. Furthermore, this project will examine whether these functionalized carbohydrates have the ability to remove phosphates from waste water. Eutrophication of waterways due to excessive nutrient levels is an important environmental issue, and it is hoped that our functionalized carbohydrates will constitute an inexpensive and effective method for phosphate removal. This presentation will discuss the synthesis and properties of functionalized carbohydrate gelators.

24. Solvothermal Synthesis and Characterization of Pristine Barium Titanate (BaTiO$_3$) and Chromium-Doped Barium Titanate Colloidal Nanocrystals

*Nilave Chakraborty, CMU*

Barium titanate, BaTiO$_3$, nanoparticles are widely known due to their excellent dielectric, ferroelectric, and piezoelectric properties. The demand for BaTiO$_3$ nanocrystals is augmenting sharply due to their advanced applications in microelectronics industries. The doping of BaTiO$_3$ (BTO) nanoparticles with Cr$^{3+}$ exhibits a combination of magnetic and electric orderings, known as multiferroics, have significant potential for high-density memory storage and the design of complex multistate memory elements. A solvothermal method was developed to synthesize well-isolated, nanocrystalline BaTiO$_3$ and Cr-doped BaTiO$_3$ with a narrow size distribution. The synthesized nanoparticles were characterized by using powder X-ray diffraction (XRD), transmission electron microscopy (TEM) and Raman spectroscopy. In addition, the properties of the nanoparticles were determined and explained according to the concentration of the dopant. Furthermore, the synthesized nanocrystals were utilized to study the measurements of the electric polarization and the coupling between the electric dipole and magnetic moments.

25. Progress Towards an $^{19}$F Magnetic Resonance Probe for Visualizing Gene Expression

*Justin Massing, UM-Flint*
Monitoring gene expression has become a routine practice in the field of molecular biology owing to the availability of numerous reporter genes. First, a gene of interest is incorporated into an organism’s genome along with a reporter gene. Successful incorporation of the gene of interest may then be monitored given some measurable output facilitated by the reporter gene chosen. For instance, the lacZ gene encodes the reporter protein β-galactosidase (β-gal), the activity of which may be monitored using commercially available X-gal. β-gal converts this colorless X-gal reagent into a blue-colored indigo derivative that is then detected visually. Unfortunately, this mode of visualizing gene expression is limited to translucent specimens or postmortem detection only. Herein we present progress towards an $^{19}$F magnetic resonance (MR) probe that would enable noninvasive visualization of gene expression in opaque specimens. Hydrolysis of a galactose residue by β-gal is expected to unmask an electron-donating phenol capable of initiating a self-immolative cascade and concomitant change in the $^{19}$F MR response.

26. Manipulating Redox Process That Affecting the Size and Antimicrobial Activity of Silver Nanoparticles

Waleed Seddiq, SVSU

In recent years synthesis of silver take up a respected part of scientific publication due to the properties of these nanoparticles including inhibition of bacteria. Different approaches like chemical synthesis and physical synthesis and they can cause a toxicity and utilized hazardous chemical, therefore, overcome the toxicity problem and using hazardous chemicals the need to utilize green synthesis based on green leaves is one of the aims of the number of studies as it is ecofriendly, inexpensive and maintains energy. Many studies show that the metal nanoparticles found to be effective against pathogenic such as bacteria with some variation in effectiveness. Some of the bacteria form a resistance from anti-biotic, and they became a primary public health problem. Bacopa monnieri (L) is a perennial creeping plant found throughout many countries including Saudi Arabia. In this study, silver nanoparticles (Ag NPs) are synthesized with green- and chemical-based redox methods. Each method’s effect on particle size is studied, as well as the potential of the produced Ag NPs to inhibit bacteria. FESEM, UV-Vis, and FTIR are used to characterize the particles, and the particle sizes are measured using a NanoSight platform. This study produces three main results: First, certain synthesis parameters create specific particle sizes; second, particle size significantly informs Ag NPs’ potential to inhibit bacteria; and third, the Ag NPs derived from the green redox method have more bacteria-inhibiting potential than the chemically synthesized ones have.

27. Catalytic Reduction of Oxyanions Using Bimetallic Nanoparticle Carbon Microsphere Composites

Slone Schultz & Mary Beall, Albion

Oxyanions are emerging contaminants because of their increasing concentration in the environment and known health impacts. One method explored for the removal of oxyanions is hydrogenation, but it is hindered by catalyst (Pt/C, Pd/C) costs. This research focuses on the development of inexpensive bimetallic catalysts for the hydrogenation of oxyanions. The catalysts are made using ultrasonic spray pyrolysis (USP), producing highly porous carbon microspheres (CM) with bimetallic nanoparticles embedded in them. To date Ni/Fe, Ni/Cu, Ni/Co, Fe/Cu, Fe/Co, and Cu/Co CMs have been made. Ni/Fe CMs show promise in the reduction of bromate. Our latest results from optimizing these systems will be presented.

28. Preparation of 2-Alkylaminomethylene Indoles and Respective Aluminum Complexes
2-Monoalkylaminomethylene and 2-dialkylaminomethylene indole ligand precursors were prepared from ethyl indole-2-carboxylate starting material. These precursors can be synthesized in large scale quantities (2.5 – 4.0g) and subsequently complexed with respective main group metals; affording complexes that have potential in ring opening polymerization (ROP), hydroamination and carbonylation reactions. Synthetic routes to ligand precursors and metal complexes will be presented with emphasis on reducing the number of synthetic steps while achieving greater ligand yield and purity.

29. From Closed-Shell to Open-Shell Biradical: Mechanochemical Breaking of a π-bond

Maude Desroches, Dow

A new quinodimethane aromatic polycyclic based on the 4,10-dibromoanthanthrone dye is reported. Acene molecules have attracted a lot of interest for the preparation of stable biradicals. While the anthanthrone core can be viewed as a fusion of two anthracene moieties with lateral functionalization, its chemical and physical properties stand in sharp contrast with the parent anthracene subunit. The anthanthrone core shows remarkable stability because of its extended delocalization. The intrinsic steric congestion of a disubstituted quinoidal anthanthrone structure leads to a biradical formation. The compound adopts a stable closed-shell structure at room temperature but can be excited to a biradical form by applying weak pressure in the solid state or increasing the temperature in solution. The steric congestion promotes π-bond breaking, resulting in the rearrangement of the butterfly-shaped quinodimethane geometry to a planar aromatic structure. We also show that the ease of biradical formation depends on the nature of the substituents located on the peripheral phenyl rings.

30. Novel Organic Molecules for Energy Storage Applications

Briana Dore¹, Rita Halphen², Christi LeCaptain³, Liam Pan⁴, Dayton Richard¹ and Adina Dumitrascu⁵

¹SVSU Great Lakes Bay Early College, ²Midland High School, ³Dow High School, ⁴Freeland High School, ⁵Michigan State University

There is a large and rapidly growing need for electrical energy storage in modern society. Lithium ion batteries (LIBs) are ubiquitous, powering everything from our cell phones to power tools, to cars. However, there are still some safety concerns, often related to the danger presented by LIB overcharge. Overcharge generally occurs when a current is forced to a cell, and the charge delivered exceeds its charge-storing capability. Overcharge of LIBs can lead to chemical and electrochemical reaction of batteries components, rapid temperature elevation, self-accelerating reactions, and even explosion. Redox shuttles additives have been used for overcharge protection for decades. Generally, they are organic molecules that undergo reversible electrochemical oxidation at potentials near the maximum design value. Many of the compounds studied to date are either too expensive or not sufficiently durable for commercial applications.

At the same time, redox-active organic materials are being investigated in order to develop nonaqueous redox flow batteries (RFBs) for inexpensive, grid-level electrical energy storage systems. Indeed, because such materials must exhibit reversible oxidation at high potential, many candidates for redox shuttles have also been employed as catholytes in RFB applications.
In this presentation, we describe ongoing efforts to develop heterocyclic systems with high oxidation potentials and very stable radical cation states for both redox shuttle and RFB applications. One part of our strategy includes “tuning” oxidation potentials by using steric factors and considering the changes in molecular geometry that occur upon oxidation. We also describe several novel trifluoromethyl-carbazole derivatives that exhibit reversible electrochemical oxidation at potentials above 4.2 V vs. Li/Li⁺ and very good solubility in carbonate solvents, making them attractive candidates both as redox shuttle additives for LIB and as catholytes in organic redox flow batteries (ORFBs) for inexpensive grid-level energy storage.
The 2019 ACS-FSM Committee Team

- Chairs: Tom Bekemeier & Elizabeth Santos, Dow
- Oral Presentation Chair: Krishna Janmanchi, Dow
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