



# Research Symposium & Industry Collaborative

Thursday, April 11, 2019

2:00 pm – 8:30 pm

University of Dayton Research Institute  
1700 S. Patterson Blvd., Dayton, OH 45409



# Welcome

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For the first time in recorded memory, the Midwest Chapter of the Society for the Advancement of Material and Process Engineering (SAMPE) and the Dayton Section of the American Chemical Society (ACS) will be teaming up to sponsor a joint effort of two of the societies' signature events for student researchers: the Student Research Symposium of the SAMPE Midwest Chapter and the Annual Poster Session of the Dayton Section of the ACS. Our goal for this event is to share and celebrate the achievements of researchers at all levels – but particularly those of local graduate and undergraduate students.

In addition to this, thanks to a generous bequest from the Patterson family, the Dayton Section of the ACS are able to award the best junior Chemistry majors from each of the schools in the area the *Patterson College Chemistry Award*. We look forward to celebrating their achievements as well. SAMPE Midwest will also be hosting an Industry Collaborative where suppliers, manufacturers, and clients will be able to collaborate and network with each other!

We look forward to meeting all of you and hope you will have a good time at this event!

# Agenda

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## SAMPE Midwest Oral Presentations - *Marshall Room*

2:00 – 2:10 PM	Sign-in & Refreshments
2:10 – 2:20 PM	<ul style="list-style-type: none"><li>• Welcome</li><li>• Introduction to the Judges</li></ul>

Master's Category	
2:20 – 2:40 PM	<b>Effect of Heat Damage on the Double Lap Joint Strength of Pultruded E-glass/Polyester Material</b> Abdalla Alomari, University of Dayton
2:42 – 3:02 PM	<b>Additive Manufactured Lattice Structures for Orthopedic Implants, Review of Mechanical Properties, Osseointegration Properties and Process Monitoring of Selective Laser Melting via Neural Networks</b> Dimitri Papazoglou, University of Dayton
3:04 – 3:09 PM	5 Minute Break

Doctoral Category	
3:09 – 3:29 PM	<b>Printed Polymer Heat Sinks for High-Power, Flexible Electronics</b> Katherine Burzynski, University of Dayton
3:31 – 3:51 PM	<b>Electrical and Thermal Properties of Graphene Reinforced Polyimide Composites</b> Wajeeh Marashdeh, University of Cincinnati
3:53 – 4:13 PM	<b>Hybrid Carbon Nano-Fibers with Improved Oxidation Resistance</b> Saja Nabat Al-Ajrash, University of Dayton
4:15 – 4:35 PM	<b>Kinetics for Homo- and Hetero-geneous Crystallization of Tungsten Selenide</b> Rachel Rai, University of Dayton
4:37 – 4:57 PM	<b>Thermal Decomposition Studies of Polyimide/Graphene/Clay Nanocomposites</b> Caroline Akinyi, University of Cincinnati
4:59 PM	End of Oral Presentations

5:00 – 6:00 PM	Dinner – <i>Meyer Room</i>
6:00 – 8:00 PM	Dayton ACS Poster Session – <i>Meyer Room</i> SAMPE Midwest Industry Collaborative – <i>Marshall Room</i>
8:00 – 8:30 PM	Awards Ceremony – <i>Meyer Room</i>

**Event Attire: Business Casual**

# About the Organizing Societies

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## Dayton Section of the American Chemical Society

The beginnings of the Dayton Section date back to 1929. The first official Chair of the Section was Dr. C. A. Thomas, who served from 1931-1932. Our current membership is about 400, covering the counties of Montgomery, Greene, Miami, Clark, Preble, and Darke. Section meetings, featuring national and local speakers, are held quarterly and include a local poster session. In addition, the last meeting of the year honors the 50-year and 60-year members.

The Section has a long history of administering local philanthropy:

- The **Patterson High School Chemistry Awards** go to winners of the Patterson High School Chemistry Competition, which consists of two stages: examination and essay. First, second, and third prizes are \$1000, \$750, and \$500. Originally established by Charles A. Thomas and Carroll A. Hochwalt, former Dayton chemists and Monsanto researchers, the top chemistry students in the area have been recognized since 1943. In 1990, the family of the late Austin M. Patterson, also a prominent Dayton chemist, assumed sponsorship.
- Recipients of the **Patterson College Chemistry Awards** are chosen by the faculty of each of the universities within the Dayton Section from their outstanding junior chemistry majors using the general criteria of scholarship, character, extra-curricular involvement, and potential for success after college. Winners receive a certificate of recognition and a check for \$400.
- The **Patterson-Crane Award** was originally established in 1949 as the Austin M. Patterson Award to acknowledge meritorious contributions to chemical literature and documentation of chemistry. Dr. Patterson was the first recipient for his work as editor of Chemical Abstracts from 1909-1914. The biennial award was expanded in 1975 to honor another Chemical Abstracts editor (1915-1958) and 1953 award recipient, E. J. Crane. The award, which includes a monetary honorarium, is now funded by a bequest of the Patterson family, by the Helen G. Crane Fund of the Columbus Foundation, and by the Patterson-Crane Award Fund of the Dayton and Columbus Sections.

The Dayton Section also participates in the **Dayton/Miami Valley TechFest, Earth Week, National Chemistry Week**, and contributes funds and judges for the **West District Science Fair**.

### Officers

Chair:	Dr. Erick Vasquez
Chair-Elect:	Dr. Prakriti Pollack
Immediate Past Chair:	Dr. Anastasie Weaver
Treasurer:	Dr. Justin Biffinger
Secretary:	Dr. David Wang
Councilor:	Dr. Steve Trohalaki
Alternate Councilor:	Dr. Yu Kay Law

Dr. Erick Vasquez also serves as the Chair of the Patterson College Chemistry Awards Committee.

# Midwest Chapter of the Society for the Advancement of Material and Process Engineering

Midwest SAMPE is a non-profit organization established in accordance with the provision of the International Chapter to be the premier, if not only, technical society in the Midwest region to encompass all fields of endeavor in materials and processes (M&P).

To achieve this purpose, Midwest SAMPE will:

- be an accessible, reliable, efficient, and effective source of technical information for the M&P community. This information will encompass both established technical knowledge and state-of-the-art technical developments regarding plastics and polymer matrix composites, metals and metal matrix composites, and monolithic ceramics and ceramic matrix composites;
- provide forums and other mechanisms that are conveniently accessible to members from the entire Chapter area for networking and the free exchange of ideas;
- be an active advocate of higher education;
- be an advocate for the advancement and application of new technologies in the M&P field.

The subgoals set forth in the Purpose Statement will be implemented and maintained in the following manners:

- Technical information will be disseminated through meetings, seminars, short courses, and a network of local engineers and scientists. However, due to the immense breadth of M&P information, Midwest SAMPE cannot and will not try to be everything.
- For those technical areas that are being more appropriately addressed by other focused societies, Midwest SAMPE will provide its membership with access via joint meetings, recommendations and advertising of other conferences, and recruiting of experts in these other societies to participate in this Chapter.
- Forums will be manifested in both in-person contact and electronic communication. Examples of the first include regular meetings and speakers, conferences, social and technical activities, and focus groups. Examples of electronic communication include email, an up-to-date web site, and video conferences.
- Midwest SAMPE will foster student chapters, offer scholarships and awards, make information and forums available to students, and encourage them to use the resources.
- Midwest SAMPE will be an advocate for the advancement and application of new M&P technologies through execution of the previous three goals and the existence of an active and prospering Midwest Chapter in general.

## Officers

Chair:	Robyn L. Bradford-Vialva	Voting Director 1:	Douglas D. Ward
Vice Chair 1:	Tom Margraf, Jr.	Voting Director 2:	Anthony E. Saliba
Vice Chair 2:	Thao Gibson	Non-Voting Director:	James Johnson
Treasurer:	Andrew Abbott		
Secretary:	Philip J. Kauffmann		

## About the Host Institution

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The University of Dayton has been affiliated with the Marianist order of the Catholic Church since its founding in 1850; and Chemistry has been taught at the University of Dayton since its founding. Certified by the American Chemical Society for over 100 years, the Department of Chemistry has eleven full-time tenure-track faculty, seven other full-time faculty, and annually graduates an average of twenty majors from its Bachelor of Science Programs in Chemistry, Biochemistry and Medicinal and Pharmaceutical Chemistry and the Bachelor of Arts Program in Chemistry. Notable alumni include the Nobel Prize winner for the discovery of crown ethers, Charles Pedersen (class of 1926); Carroll Hochwalt (class of 1920), inventor of the first practical chemical fire extinguisher; and Charles Maggati (class of 1971), co-discoverer of the drug Claritin.

The Dayton Section of the ACS and the Midwest Chapter of SAMPE thanks Provost Paul Benson, Dean of the College of Arts and Sciences Jason Pierce, Chemistry Department Chair David Johnson, the School of Engineering, and the University of Dayton Research Institute as well as all the faculty and students of the University of Dayton for welcoming, hosting, and providing support for the Joint Research Symposium and Industry Collaborative.

## Patterson College Chemistry Awards

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The Patterson College Chemistry Awards are administered by the Dayton Section of the American Chemical Society and are presented annually to outstanding junior chemistry majors at each university within the Section's boundaries. This year, the awardees are:

Kelsy Boyes	Cedarville University
Morgan Grunden	Wright State University
Katie Robinson	Wittenberg University
Alexis Smith	University of Dayton

### Kelsy Boyes, Cedarville University

Kelsy Boyes is an undergraduate Chemistry major at Cedarville University, class of 2020. She grew up moving all around Ohio in the "scenic tour" before graduating from Lima Shawnee High School. During her time at Cedarville, she has taken part in research and is an active member of the ACS chemistry club student chapter on campus. She served as treasurer during the 2017-2018 school year and president during the 2018-2019 school year. Her research involvement at Cedarville includes organic synthesis and polymer chemistry projects with Dr. Hnatiuk and Dr. Sekerak. Last summer she was selected to participate in the Nuclear Chemistry Summer School at Brookhaven National Lab on Long Island in New York. During her time there, she was trained in techniques working with radioactive materials and got a close look at several amazing facilities including the NASA Space Radiation Lab, the National Synchrotron Light Source II, and the Relativistic Heavy Ion Collider. This experience opened her eyes to new fields of chemistry applications. She is also the recipient of the Heyd Science and Math Award. Her favorite classes include Advanced Inorganic Chemistry and Analytical Chemistry. She loves taking all of the extra Bible classes she can fit into her schedule, and especially enjoyed learning New Testament Greek. This summer she will do inorganic research under Dr. Fieser at the University of Southern

California. After graduation she wants to pursue a Doctorate in inorganic chemistry. In her free time, Kelsy enjoys leading a team that holds conversational English classes for foreign students, directing review sessions for general chemistry students, running, and reading anything she can get her hands on.

## Morgan Grunden, Wright State University

Morgan Grunden is a junior Chemistry major at Wright State University. She graduated from Coldwater High School in 2016. In high school, she took two years of chemistry including AP Chemistry. Her high school chemistry teacher sparked her interest in chemistry and pushed her to excel. After high school, Morgan enrolled at Wright State University in the fall of 2016. She completed two years of classes at the Wright State University Lake Campus. Once she completed Organic Chemistry at the Lake Campus, she started taking classes at Wright State University in Dayton in the summer of 2018. Morgan has plans to begin undergraduate research at Wright State this coming fall. After graduating in the spring of 2020 with an ACS Certified Bachelor of Chemistry, Morgan intends to continue her education at Wright State to pursue a Master of Science in Chemistry. When Morgan is not studying or in class, she enjoys spending time with her family and friends, playing with her dog, reading, and watching or playing sports. She is enjoying her time at Wright State and is excited to see where the future takes her.

## Katie Robinson, Wittenberg University

Katie is from the Springfield area. She attended the Dayton Regional STEM school for her first two years of high school before transferring to Sidney High School to start taking college level classes through Ohio's CCP program. She is double majoring in Chemistry and Physics, and has performed undergraduate research in both areas. First, she examined the energetics of sugars binding to proteins using computational chemistry at Wittenberg University. Next, she studied thin-films using the Magneto-Optical Kerr Effect at the Ohio State University. She plans to attend graduate school after finishing at Wittenberg.

## Alexis Smith, University of Dayton

Alexis Smith is a junior Medicinal-Pharmaceutical Chemistry major at the University of Dayton. She is from Lancaster, Ohio and began to have an interest in chemistry in her junior year of high school. At the University of Dayton, she has continued to develop and share her enjoyment of chemistry through various activities. She is a private tutor for general chemistry students and was an undergraduate general chemistry lab Teaching Assistant last fall, which she hopes to continue next year. Alexis has been working in a faculty research lab since her sophomore year with Dr. Judit Beagle, and last summer was a member of the Integrated Science and Engineering Summer Corps where she worked on a collaborative project with three chemistry faculty members investigating the role of chromophore isomerization in the laser-induced color change in bacteriorhodopsin. She plans to return this summer as a Dean's Summer Fellow to continue to research this project and will be using the collected data to write her Honors Thesis this upcoming year.

Alexis is also involved with many activities outside of the lab. She is the Treasurer of the University of Dayton's student chapter of the ACS and the President of the University of Dayton Swing Dance Club where she also volunteers as an instructor each week. She enjoys playing the flute and does so in the University of Dayton Concert Band as well as playing for Mass at the Chapel of the Immaculate Conception most Sundays in the school year. Alexis plans to go to graduate school to further her education, focusing on organic chemistry.

# Oral Presentation Abstracts

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## SAMPE Midwest Chapter Student Research Symposium

All presenters will earn cash awards. In addition, the first-place graduate winner receives an all-expenses paid trip to compete at the national level at CAMX 2019 in September in Anaheim, CA upon submission of a paper.

### Masters Category

Oral Presentation 1 (2:20 – 2:40 pm)

#### **Effect of Heat Damage on the Double Lap Joint Strength of Pultruded E-glass/Polyester Material**

Alomari, A.W.\*<sup>1</sup>, Toubia, E.A.\*<sup>1</sup>, Morgan, B. A.\*<sup>2</sup> and Klosterman, D.\*<sup>1</sup>

<sup>1</sup>University of Dayton, <sup>2</sup>University of Dayton Research Institute

A comprehensive experimental investigation was conducted to study the effect of post-heat damage on fire retardant glass fiber-reinforced pultruded members. A total number of 63 double lap shear joints were tested. The test parameters included: 1) flat plate thickness (6 and 12 mm); 2) heat induced damage using the cone calorimeter test (10 and 20 Kw/m<sup>2</sup>); and 3) fiber orientation (0, 45 and 90°) with respect to the member's pultrusion axis. The test results revealed that for the thin plate (6 mm thick) the maximum strength reduction (around 20%) occurred when the load is applied along the 0° fiber direction. This was justified using post-mortem digital microscopic and SEM images where a significant delamination and fiber buckling occurred at the bearing location of the bolt. In addition, a change in failure mode was observed for the higher heat flux, where the failure mode shifted from shear-out/ bearing to shear-out/bearing and net tension. The strength reductions of the double lap shear joints with 45 and 90° fiber orientation with respect to the load were 18% and 14%, respectively. For both plates' thicknesses, net tension failure mode was the dominant mode for the 45 and 90° off-axis loaded joints. This presentation also presents the temperature profile and degradation through the thickness of the damaged pultruded plates, in addition the mean strains with the loads. Also, the variation of the experimental and predicted loads, modulus of elasticity, tensile failure strain, and tensile strength are investigated.

Oral Presentation 2 (2:42 – 3:02 pm)

#### **Additive Manufactured Lattice Structures for Orthopedic Implants, Review of Mechanical Properties, Osseointegration Properties and Process Monitoring of Selective Laser Melting Via Neural Networks**

Papazoglou, D.\*<sup>1</sup>, Amy, D.<sup>1</sup>, Subramanyam, G.<sup>1</sup> and Erdahl, D.<sup>2</sup>

<sup>1</sup>University of Dayton, <sup>2</sup>University of Dayton Research Institute

The call for orthopedic implants is a growing concern with an ever-rising aging population. Current orthopedic implants provide good mechanical strength and stability, with some offering surface area bone growth. Lattice structures manufactured via additive manufacturing offer patient specific orthopedic implants with viscoelastic properties similar to bone, less weight and promotion of internal bone growth for better fixation. Two different lattice structures of cubic and diamond were printed in Ti-6Al-4V via an open architecture selective laser melting machine. These lattice structures varied in pore size of 400, 500, 600 and 900µm. Compression and tensile testing were performed to identify mechanical properties like bone. Properties needed to promote osseointegration are reviewed, such as pore size and geometry. A convolutional neural network is employed

to detect defects and geometries during selective laser melting process. Identifying defects and geometries is called process monitoring. Combining process monitoring, along with non-destruction evaluation such as computer tomography scanning and scanning electron microscope techniques, can insure high quality and defect free parts for biomedical and aeronautical applications.

## Doctoral Category

Oral Presentation 3 (3:09 – 3:29 pm)

### **Printed Polymer Heat Sinks for High-Power, Flexible Electronics**

Burzynski, K.M.<sup>\*1,2</sup>, Glavin, N.R.<sup>1</sup>, Heller, E.R.<sup>1</sup>, Snure, M.<sup>3</sup>, Heckman, E.M.<sup>3</sup> and Muratore, C.<sup>2</sup>

<sup>1</sup>*Air Force Research Laboratory, Materials and Manufacturing Directorate, WPAFB, OH 45433 USA*

<sup>2</sup>*University of Dayton, Department of Chemical and Materials Engineering, Dayton OH 45409 USA*

<sup>3</sup>*Air Force Research Laboratory, Sensors Directorate, WPAFB, OH 45433 USA*

Consumers and military personnel alike are demanding ubiquitous electronic devices which require enhanced flexibility and conformality of electronic materials and packaging, while maintaining device performance. Whether it be high-power devices for faster data speeds, such as fifth generation (5G) wireless communication technology or wearable sensors to facilitate the Internet of Things (IoT), the age of flexible, high performance electronic devices has begun. Managing the heat from flexible electronics is a fundamental challenge. Even on rigid substrates with significantly higher thermal conductivity than polymeric and other flexible substrates, the full potential of semiconducting materials is often thermally limited. The flexible gallium nitride (GaN) high electron mobility transistors (HEMTs) employed in this work are conventionally processed devices that can be released from their growth substrate and transferred to a variety of rigid and flexible substrates. Characterization of the GaN device behaviour on the as-grown sapphire wafers (prior to transfer) provide a baseline for evaluation of the thermal performance of engineered interfaces and substrates. With conventional substrates, device performance (specifically, the saturation current) is reduced when the device is transferred to polymeric substrates. The thermal dissipation is further restricted due to the addition of an adhesive layer to the substrate. Thermal imaging of devices in operation reveals that the current passing through an as-grown GaN transistor on a sapphire wafer reaches the target operating temperature at approximately five times the power of the same device transferred to a flexible substrate. Printable, thermally conductive nanocomposites integrating 1D, 2D, and 3D forms of carbon in a flexible polymer matrix, as well as metal nanoparticles, were developed to maximize heat transfer from electronic devices. The thermal conductivity of the candidate substrate materials was measured experimentally to have more than a 900 percent increase in thermal conductivity (from 0.2 to 1.7 W/mK), while maintaining desirable mechanical properties. The performance of devices transferred to these novel flexible composite substrates was characterized and used in computational simulations to predict flexible substrate architectures that effectively promote point-to-volume heat transfer to further improve device performance. Additive manufacturing for engineered architectures of the flexible, thermally conductive substrate materials was demonstrated to substantially reduce the thermal limitation of high-power flexible electronics.

Oral Presentation 4 (3:31 – 3:51 pm)

**Electrical and Thermal Properties of Graphene Reinforced Polyimide Composites**

Marashdeh, W.F.\*<sup>1</sup> and Iroh, J.O.<sup>1</sup>

<sup>1</sup>*Department of Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, Ohio 45221*

Polyimide graphene composites were synthesized by an in-situ polymerization using Pyromellitic dianhydride, Oxydianiline, nanographene sheets and Polylactic acid. AC-conductivities, dielectric permittivity ( $\epsilon'$ ) and dielectric loss ( $\epsilon''$ ) of polyimide graphene composite and pure polyimide have been measured in the temperature range from 30°C to 200 °C and frequency range from 200 to 20 kHz. The results imply that the increase of the volume fraction of graphene up to 10%, resulted in an extremely large increase in the dielectric constant. The electrical conductivity of the composite is higher than pure polyimide by six order of magnitude and it is attributed to the formation of conducting paths in the matrix by the graphene sheets. Also, this study showed that the thermal conductivity of the composites increased sharply with increasing graphene concentration. Porous polyimide graphene composite having porous structure was prepared by thermal decomposition and extraction of poly lactic acid (PLA) introduced into the composite during synthesis. The presence of pores increased available surface area available for electrical charges adsorption and double layer formation.

Oral Presentation 5 (3:53 – 4:13 pm)

**Hybrid Carbon Nano-Fibers with Improved Oxidation Resistance**

Nabat Al-Ajrash, S.M\*<sup>1</sup> and Lafdi, K.<sup>1</sup>

*Dept. of Chemical and Materials Engineering, University of Dayton, 300 College Park, Dayton, OH 45469, USA*

Hybrid Carbon-Silicon Carbide (C-SiC) nano-fibers were fabricated while using a mixture of polyacrylonitrile (PAN) and silicon (Si) nanoparticles as precursors. The microstructure of the material was examined using X-ray diffraction and Raman spectroscopy as a function of processing temperature and holding time. A complete transformation of Si to SiC occurred at 1250 °C. However, for heat treatments below 1000 °C, three distinct phases, including Si, C, and SiC were present. The effect of microstructural changes, due to the heat treatment, on oxidation resistance was determined using thermogravimetric analysis (TGA). Furthermore, the char yield showed exponential growth with increasing the carbonization temperature from 850 °C to 1250 °C. The holding times at higher temperatures showed a significant increase in thermal properties because of SiC grain growth. At longer holding times, the SiC phase has the function of both coating and reinforcing phase. Such structural changes were related to fibers mechanical properties. The tensile strength was the highest for fiber carbonized fibers at 850 °C, while the modulus increased monotonically with increasing carbonization temperature.

Oral Presentation 6 (4:15 – 4:35 pm)

**Kinetics for Homo- and Hetero-genous Crystallization of Tungsten Selenide**

Rai, R. <sup>\*1,2</sup>, Rao R. <sup>2,3</sup>, Wheeler, R. <sup>2,3</sup>, Glavin, N. <sup>2</sup>, Jawaid, A. <sup>2,3</sup> Bissell, L. <sup>2</sup> and Muratore, C. <sup>1</sup>

<sup>1</sup>*Department of Chemical and Materials Engineering, University of Dayton, Dayton OH 45469*

<sup>2</sup>*Materials and Manufacturing Directorate, Air Force Research Laboratories, WPAFB, OH 45433*

<sup>3</sup>*UES, Inc. Dayton OH 45432*

Single to few-layered Group-VI semiconducting transition metal dichalcogenides (TMD) are new materials that exhibit versatile physical properties, such as sizable direct band gaps, that promise new potential for many electronic and optoelectronic devices. A prototypical TMD, tungsten selenide (WSe<sub>2</sub>) exhibits captivating properties such as room temperature photoluminescence. However, the integration of WSe<sub>2</sub> and other TMDs into devices is currently limited due to the inaccessibility of scalable techniques to fabricate high quality large area thin films. This impediment can be resolved by understanding and optimizing the kinetics of film growth. Thus, our work encompasses innovative techniques to study the crystallization kinetics of thin amorphous homo- and hetero-genous films of WSe<sub>2</sub>. We begin by sputtering thin amorphous films of WSe<sub>2</sub> on flexible and rigid substrates. We then crystallize the deposited films by supplying enough energy for crystallization via broadband radiation, nanoscale beams, and *in-situ* Raman Spectroscopy. Magnetron sputtering is selected as the deposition technique due to the low temperatures involved, thus allowing deposition on polymer substrates. Furthermore, modulation of the energy flux during magnetron sputtering provides an opportunity to model homo- or hetero-geneous crystallization by forbidding or permitting the presence pre-existing nuclei, respectively. Our employment of various crystallization techniques allows for methodical study of the influences of seeds on 2D nucleation and growth kinetics. Results show that homo-geneous crystallization has a lower nucleation due to the small seed size. Such finding is systematically explained by crystallization theories that relate the critical radius size of the seeded materials to energy barriers. The newly founded relationship between deposition parameters, activation barriers, and film quality of WSe<sub>2</sub> is applicable to other TMDs. Thus, our work significantly contributes to the advancement TMDs and eases their incorporation in future electronic devices.

Oral Presentation 7 (4:37 – 4:57 pm)

**Predicting Flammability Behavior of Polyimide/Graphene Nanocomposites  
Using Thermoanalytical Data Obtained from DSC and TGA**

Akinyi, C. <sup>\*1</sup> and Iroh, J.O. <sup>1</sup>

<sup>1</sup>*Department of Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, Ohio 45221*

Thermoanalytical data obtained from differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) was used to quantify the thermal stability and combustion properties of neat polyimide and polyimide-graphene composites. The presence of graphene resulted in a remarkable decrease in the heat of combustion of the polymer by up to 81% at 50 wt.% graphene. The heat release capacity was used to predict the flame resistance and fire performance of the neat polymer and the composites. An increase from 0- 50 wt.% graphene led to a 77% decrease in HRC indicating that the presence of graphene contributed to the increase in anti-flammability behavior of polyimide. The decrease in HRC slowed down at 30 wt.% graphene, showing only a 2.7% decrease between 30 wt.% and 50 wt.%. The rate of degradation was also shown to significantly decrease

by up to 85% from 0-50 wt.% graphene. There was a 47 % improvement in char retention at 50 wt.% graphene. The rate of mass loss was also remarkably decreased by 45 % at 50 wt.% graphene. This attested to the powerful shielding properties of graphene, creating a barrier that protects the polymer from the heat source.

## ACS Annual Poster Session

The posters are listed below by presenter category. Graduate and undergraduate student posters will be judged and the best posters in each category will be awarded cash prizes at the award ceremony at the end of the event.

### Professional Chemists

Poster No. 1

#### **Development of Liquid Crystalline Thermosets for Additive Manufacturing**

Trigg, E.B.\*; Koerner, H.

*Air Force Research Laboratory; Polymer Matrix Composites Group*

The additive manufacturing (AM) of high-temperature thermosetting resins would enable rapid functional prototyping and on-demand production of high-performance aircraft parts; however, limitations of current feedstock materials have prevented AM of such parts to date. The use of liquid crystalline thermosets could overcome several critical challenges in fused deposition modeling, such as tuning the rheology during print and cure to improve mechanical properties of printed parts. The shear-alignment of liquid crystal domains by the nozzle could also allow for the controlled design of anisotropic properties. Here, thermosetting systems (epoxies, polyimides) are studied with respect to AM processing. Crosslink topology is controlled using several curing agents to tune the rheology and gelation time. We study the cure reaction in detail using in situ methods including FTIR, Raman, X-ray scattering, and XPCS.

### Graduate Researchers

Poster No. 2

#### **Chemically Fueled Covalent Crosslinking of Polymer Materials**

Borui Zhang,\* Isuru M. Jayalath, Jun Ke, Jessica L. Sparks, C. Scott Hartley and Dominik Konkolewicz  
*Department of Chemistry and Biochemistry, Miami University, Oxford, Ohio 45056; and Department of Chemical, Paper and Biomedical Engineering, Miami University, Oxford, Ohio 45056*

The use of chemical fuels in nonequilibrium assembly is ubiquitous in nature but much less common in abiotic systems. Here, chemically fueled and transiently crosslinked polymer materials were synthesized using the hydration of carbodiimides to link pendant carboxylic acids as anhydrides. Our design is based on simple acrylamide and acrylic acid copolymers. The covalent crosslinking was fueled using EDC. Beginning with aqueous polymer solutions, we observe the formation of hydrogels, which dissolve as the anhydrides are hydrolyzed. Both the mechanical properties and lifetimes of the gels are determined by the proportion of acid groups in the starting polymers. The gels exhibit higher storage moduli compared to previously reported transient supramolecular gels as a result of their covalent cross-links. The polymers can also undergo subsequent refueling cycles to regenerate the gel state. Small molecule, macroscopic and rheological

properties of this reaction were investigated, showing that this is a powerful platform for materials which need temporary changes in mechanical properties.

Poster No. 3

**Utilizing RAFT Polymerization and Dynamic thiol-Michael Chemistry for Tunable Thermoresponsive Dynamic Polymer Networks**

Progyateg Chakma, Zachary A. Digby, Jeremy Via, Max P. Shulman, Jessica L. Sparks and Dominik Konkolewicz  
*Department of Chemistry and Biochemistry, Miami University, Oxford, OH; and Department of Chemical, Paper and Biomedical Engineering, Miami University, Oxford, OH*

Polymeric materials crosslinked with exchangeable bonds have received significant interest due to unique properties such as re-healability, shape-memory, malleability, and degradability. The thiol-Michael reaction (TM) is reported to be dynamic at elevated temperatures and pH values and recently has been utilized in developing self-healing and malleable materials via free radical polymerization (FRP), although resulting in uncontrolled macromolecular architecture. The effect of polymer architecture utilizing well-defined thiol polymer on the self-healing properties of the materials has not been investigated yet. This work reports synthesis of a series of well-defined thiol polymers utilizing reversible addition-fragmentation chain transfer (RAFT) polymerization and then post-polymerization crosslinking using the TM reaction for thermoresponsive self-healing, malleable, and mechanically stable materials.

Poster No. 4

**Hybrid Carbon Nano-Fibers with Improved Oxidation Resistance**

Saja M. Nabat Al-Ajrash and Khalid Lafdi  
*University of Dayton*

Hybrid Carbon-Silicon Carbide (C-SiC) nano-fibers were fabricated while using a mixture of polyacrylonitrile (PAN) and silicon (Si) nanoparticles as precursors. The microstructure of the material was examined using X-ray diffraction and Raman spectroscopy as a function of processing temperature and holding time. A complete transformation of Si to SiC occurred at 1250 °C. However, for heat treatments below 1000 °C, three distinct phases, including Si, C, and SiC were present. The effect of microstructural changes, due to the heat treatment, on oxidation resistance was determined using thermogravimetric analysis (TGA). Furthermore, the char yield showed exponential growth with increasing the carbonization temperature from 850 °C to 1250 °C. The holding times at higher temperatures showed a significant increase in thermal properties because of SiC grain growth. At longer holding times, the SiC phase has the function of both coating and reinforcing phase. Such structural changes were related to fibers mechanical properties. The tensile strength was the highest for fiber carbonized fibers at 850 °C, while the modulus increased monotonically with increasing carbonization temperature

Poster No. 5

**Characterizing the structure and dynamics of styrene-maleic acid copolymer-lipid nanoparticles (SMALPS) as a membrane mimetic**

Burridge, K.M.\*; Sahu, I.D., Harding, B.D.; Bali, A.P.; Dolan, M.; Zhang, R.; Frantz, N.D.; Al-Abdul-Waheed M.S.; Dabney-Smith, C.; Konkolewicz, D.; Lorigan, G.  
*Miami University, Department of Chemistry and Biochemistry*

Membrane proteins are challenging species to study. Much work in the field has employed micelles, bicelles, and liposomes; each has unique benefits and drawbacks. Polymer-bound lipid nanodiscs (SMALPs) are an emerging technology which enable the use of a wider variety of bilayer-forming lipids, and are small enough to afford suitable samples for magnetic resonance techniques. They have also proved useful in membrane protein purification. Commercially available copolymer (styrene-maleic anhydride, SMA) for making SMALPs is often cost-prohibitive (over \$1000/g). Our group synthesizes SMA at multigram scale at a cost of dollars per gram. Recent work in our group has employed spin labels and electron paramagnetic resonance (EPR) to assess the effects of SMALPs on the dynamics of each component in the system.

Poster No. 6

### **Chemiluminescence Driven Polymerization of Acrylamide**

De Alwis N. T., Allegrezza M. L., Dolan M. T., Kloster A. J., Kovaliov M., Averick S., Konkolewicz D.  
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Recently, many photo-chemically driven reactions have been identified in the field of chemistry due to its simplicity, efficiency, and specificity. Photochemistry can be considered as a good alternative to carry out thermally sensitive reactions. In almost all the cases, photons are being supplied from external light sources by penetrating through reaction vessels. Owing to the poor penetration ability of light waves, and reflection losses sometimes causes poor photon transfer through reaction media. Hence, some photo chemically driven reactions are not being performed with their full efficacy. These limitations of external light sources emphasize the necessity of using internal light source to drive a reaction. Chemiluminescence is a process of releasing photons through a chemical reaction. This process can be found in natural environments such as bacteria, insects and human cells. Thus far, chemiluminescence have been employed in many biomedical, analytical processes and as commercialized substances such as glow sticks. The chemistry behind the glow stick is generation of high energy intermediate and transferring its energy to a fluorescence material to generate photons. The chemiluminescence reaction creates is both fascinating but also potentially useful since it generates potentially useful photons. Hence, this simple chemiluminescence reaction could be used as an internal light source to drive chemical reactions by the selection of proper biphasic systems. In this project, we have used chemiluminescence and polymer biphasic system to demonstrate that chemiluminescence can be used as an internal light source to generate photons and drive chemical reactions. Acrylamide polymerization kinetics were explored in aqueous media with the presence of a water soluble photo initiator where it sits on top of a chemiluminescence phase and absorb photons to initiate polymerization.

Poster No. 7

### **Reaction and Reactor Conditions: How Vessel Geometry and Light Source Intensity Affect Photoinduced RAFT Polymerization**

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To better understand how reaction volume and vessel geometry, as well as light source intensity impact bench-scale photochemical reactions, variations to these conditions were investigated on model photo-induced electron/energy transfer reversible addition-fragmentation chain transfer (PET-RAFT) polymerizations. By studying the kinetics of PET-RAFT in variously sized cylindrical vessels, path length for the light source was able to be varied. This showed no significant change in rate of polymerization as a result of the change in reaction vessel dimensions, suggesting that at normal bench scale, reaction vessel size and shape may be inconsequential. The intensity of the photo-reactor proved to be the most important factor, with an approximate 1/2 order scaling of the apparent rate with the intensity of the reactor, highlighting the importance of the type of light source. Reactant concentrations were also varied to better understand their roles in this photochemical process. Apparent rate of polymerization was shown to increase with catalyst loading, leveling off at higher concentrations possibly due to the optical density of the photo-catalyst.

Poster No. 8

### **Lead Discovery for Pancreatic Cancer Therapy using Privileged Chalcone Scaffold**

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K-Ras is an important signaling protein found within cells that are responsible for growth and proliferation. Mutated, or oncogenic, K-Ras can provide signaling for constant cell division and can lead to cancer. Oncogenic K-Ras has been found in 95% of all pancreatic, 45% of all lung, and 30% of all colon cancers. Additionally, there are no current drugs that target oncogenic K-Ras available on the market. Since K-Ras must interact with the plasma membrane (PM) for its biological activity, chemical compounds which are able to dissociate K-Ras from the PM could be a good starting point for developing anti-K-Ras therapeutics. This goal of this project was to examine if a lead compound capable of exerting this effect might be identified utilizing a small library of molecules from the privileged chalcone class.

Poster No. 9

### **Using Multiwall Carbon Nanotube Composites to Enhance Dynamic Properties of RAFT Polymers through Surface Diels-Alder Chemistry**

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When it comes to developing a dynamic polymer, it is important to be able to control how that material is made on a molecular level and just as important to study its performance under various conditions. One method of controlling polymer architecture is through a method called Reversible Addition Fragmentation Chain Transfer (RAFT) Polymerization, which allows the molecular weight of a material to be controlled from 1,000 g/mol to 100,000 g/mol. When the molecular weight and structure of a polymer is controlled, the functionality applications of that polymer is much greater. Polymer materials alone however, are very limited regarding mechanical and electrical properties. Recently, carbon nanotubes (CNTs) have been found to possess extremely attractive mechanical and electrical properties. They are either a single-walled or multi-walled U-shaped material, composed of a strongly bonded network of carbon atoms. This research project focuses on adding multiwalled CNTs to the controlled polymer matrix through Diels-Alder chemistry, to enhance dynamic properties including toughness, strength, and electrical conductivity. Once the crosslinked polymer is

synthesized, these dynamic materials demonstrate self-healing properties after being cut in half and heated for a certain amount of time. The materials then undergo tensile tests. Polymers in the presence of CNTs demonstrate the ability to undergo a higher amount of stress (kPa) than those polymers absent of CNTs. This trend follows for self-healing material as well. The polymers in the presence of CNTs also have greatly enhanced electrical conductivity. Adding CNT reinforcements to enhance dynamic properties of RAFT polymers will improve material strength, toughness, and electrical conductivity.

Poster No. 10

### **Colloidal Silver Nanoparticles: A more effective bactericidal agent than chlorine against waterborne Gram negative bacteria**

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The main aim of this study was to determine the antimicrobial and bactericidal activity of unfunctionalized, silver nanoparticles (eAg) of ~10 nm in diameter against well-established water-borne organisms: *Escherichia coli*, *Klebsiella variicola*, and *Pseudomonas aeruginosa*. This was achieved by determining the Minimum Inhibitory Concentration (MIC) and Minimum Bactericidal Concentration (MBC) of eAg, which were synthesized electrochemically, size-selected, concentrated, and purified by tangential flow filtration. The MIC values for *E. coli*, *K. variicola*, and *P. aeruginosa* were 0.75-4.02, 1.09-4.08, and 1.55-5.39 mg/L, respectively. The MBC values for the same bacteria were 1.51-3.96, 1.55-5.39, and 2.18-4.99 mg/L, respectively. When tested against chlorine, the MIC values increased 1000-, 2000-, and 3000-fold, respectively, for the mentioned bacteria. The MBC values increased 1000-, 1500-, and 1500-fold, respectively.

Poster No. 11

### **Enabling High-Power Flexible Devices through Tailored Nanocomposite Interface Materials**

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Consumers and military personnel alike are demanding ubiquitous electronic devices which require enhanced flexibility and conformality of electronic materials and packaging, while maintaining device performance. Managing the heat from flexible electronics is a fundamental challenge. Even on rigid substrates with significantly higher thermal conductivity than polymeric and other flexible substrates, the full potential of semiconducting materials is often thermally limited. The flexible gallium nitride (GaN) transistors employed in this work are conventionally processed devices that can be released from their growth substrate and transferred to a variety of rigid and flexible substrates. Characterization of the GaN device behavior on the as-grown sapphire wafers provide a baseline. Thermal imaging of devices in operation reveals that the current passing through an as-grown GaN transistor on a sapphire wafer reaches the target operating temperature at approximately five times the power of the same device transferred to a flexible substrate. Printable, thermally conductive nanocomposites were developed to maximize heat transfer from electronic devices. The thermal conductivity of the candidate substrate materials was measured experimentally to have more than a 800

percent increase in thermal conductivity (from 0.2 to 1.6 W/mK), while maintaining desirable mechanical properties. The performance of devices transferred to these novel flexible composite substrates was characterized and used in computational simulations to predict flexible substrate architectures that effectively promote point-to-volume heat transfer to further improve device performance. Additive manufacturing for engineered architectures of the flexible, thermally conductive substrate materials was demonstrated to substantially reduce the thermal limitation of high-power flexible electronics.

Poster No. 12

**Photonicallly annealed two dimensional transition metal dichalcogenide transducers for bioelectronic sensing**

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Typically, elastic modulus is linked to electronic bandgap in semiconducting materials, which is a primary challenge in the development of flexible electronic devices. Ultra-thin transition metal dichalcogenides demonstrate mechanical flexibility and, also, have large band gaps (1.0-2.1 eV), which enhances the response to chemical adsorption events. This unique combination of mechanical and electronic properties makes 2D TMDs attractive candidates for sensor transducers in diverse wearable sensor applications. In this work, a novel laser processing technique for large area fabrication of sensor arrays was investigated. The total laser influence was optimized by analyzing the defect density within the MoS<sub>2</sub>, in addition to the crystalline domain size and degree of crystallization. Device quality was strongly dependent on the order of device fabrication steps. Using an optimized series of fabrication steps, a flexible MoS<sub>2</sub> sensor built on a Willow Glass substrate for acetone was demonstrated to have sensitivity comparable to pristine mechanically exfoliated MoS<sub>2</sub> sensors at 100 ppm. This finding is technologically significant as the fabrication process is scalable over large areas for mass production of sensor devices.

Poster No. 13

**Computational Estimation of the Gas-Phase and Aqueous Acidities of Carbon Acids**

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A hydrogen directly attached to a carbon atom is generally not considered very acidic (i.e. ~48 for methane and other unsubstituted alkanes). However, the acidity of these compounds can be greatly increased due to neighboring electron-withdrawing substituents, hybridization effects, and resonance or aromatic effects. Carbon acids present a unique class of compounds whose pK<sub>a</sub> values span a wide range and are of importance in organic synthesis and biological chemistry. Thus, a predictive model that could estimate the acidities of carbon acids in the gas phase or in aqueous media would be of interest. Semi-empirical AM1 and Density Functional Theory (B3LYP/6-31+G\*\*) geometry optimization calculations were performed both in the gas phase and using the SM8 solvent model in aqueous solution to yield ground state Gibbs energies and total energy values for the neutral and deprotonated species of each carbon acid in this study. The calculated gas phase  $\Delta G^\circ$  values were compared to those available in NIST for the deprotonation reactions and recorded as gas phase acidities. Then, a QSAR model was developed that correlates the experimental aqueous pK<sub>a</sub> values

of 38 simple carbon acids to a molecular descriptor ( $\Delta E(H_2O)$ ), yielding  $R^2 = 0.9647$ . The final QSAR model was then used to estimate the aqueous pKa values of other carbon acids not readily available in literature.

Poster No. 14

### **Crystallization Kinetics of Amorphous WSe<sub>2</sub> and WS<sub>2</sub>**

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Single to few-layered Group-VI semiconducting transition metal dichalcogenides (TMDs) are new materials that exhibit versatile physical properties, such as sizable direct band gaps, that promise new potential for many electronic devices. The integration of TMD into devices, however, is currently limited due to the inaccessibility of scalable techniques to fabricate high quality large area thin films. Thus, our work encompasses innovative techniques to study the crystallization kinetics of thin amorphous homo- and hetero-geneous films of TMDs. We begin by sputtering thin amorphous films of tungsten based (WX<sub>2</sub>) TMDs (tungsten selenide and tungsten sulfide). We then crystallize the deposited films by supplying enough energy for crystallization via broadband radiation, nanoscale beams, and in-situ Raman Spectroscopy. Magnetron sputtering is selected as the deposition technique due to the low temperatures involved, thus allowing deposition on polymer substrates. Furthermore, modulation of the energy flux during magnetron sputtering provides an opportunity to model homo- or hetero-geneous crystallization by forbidding or permitting the presence of pre-existing nuclei, respectively. Our employment of various crystallization techniques allows for methodical study of the influences of seeds on 2D nucleation, growth kinetics, and film properties. Results show that homogeneous crystallization has a lower nucleation due to the small seed size, correlating well to classic crystallization theories. Our employment of post and in-situ processing techniques to understand crystallization and customization of properties WX<sub>2</sub> film is applicable to other TMDs, and thus significantly contributes to their advancement and incorporation in future electronic devices.

Poster No. 15

### **Effect of Geometrical Isomerism on the Thermal and Photophysical Properties of Difluorobenzophenone TADF Chromophores**

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The synthesis of thermally activated delayed fluorescence (TADF) chromophores and their incorporation into poly(arylene ether)s, PAE, were explored. Two benzophenone derivatives, 2,4-difluorobenzophenone and 3,5-difluorobenzophenone, were successfully functionalized with a carbazole donor group, via a copper-catalyzed C-N coupling reaction. Structural characterization was provided by NMR spectroscopy, GC/MS, and elemental analysis. The chromophores were covalently incorporated, at various molar ratios, into PAE systems by copolymerization with 4,4'-difluorodiphenylsulfone (DPS) and 4,4'-dihydroxydiphenyl ether (DPE) via nucleophilic aromatic substitution (NAS) chemistry. All polymeric materials synthesized provided sufficient molecular weights to cast durable films, and also possessed good thermal stability. The 2,4- and 3,5- derivatives displayed  $T_{d-5\%}$  values of 448°C and 396°C respectively, and  $T_g$  values of 177°C and 183°C respectively.

Monomer fluorescence emission peaks were quite similar for the 2,4- and 3,5- chromophores with emission occurring in the blue region at 433 nm and 446 nm, respectively. After incorporation into the P°C AE, the 3,5- derivatives produced a relatively intense emission centered around 470 nm, while the 2,4- derivative gave considerably weaker emission, which was blue shifted by ca. 30 nm.

Poster No. 16

### **Direct Ink Writing of Modified Cellulose Nanocrystals**

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Cellulose nanocrystals (CNCs) are stiff, lightweight rod-shaped nanoscale materials that have a tensile strength 8x that of steel (7.5 GPa). The addition of CNCs into a polymer matrix has been shown to enhance the mechanical properties of the resulting composite, however, the utilization of CNCs in more common non-polar polymers is still limited to their hydrophilicity and poor dispersibility. In order to fully realize the potential of CNCs as a mechanical reinforcement, it is important to modify the hydroxyl rich CNC surface. In this work we characterize the effects of a functionalized CNC on the rheological properties and printing behavior (Direct Ink Writing (DIW)) of an epoxy resin. CNC functionalization is achieved by grafting an activated medium chain fatty acid to substitute the -OH groups. The level of CNC modification is evaluated using Fourier Transform Infrared (FTIR). Functionalized CNCs are dispersed into EPON 828 at loadings up to 20wt%. Initially, rheological studies are used in this study to assess the printability of the inks. The rheological percolation threshold is the critical concentration at which there is a transition from liquid-like to solid-like behavior. For this system, this value was found to be at ~10wt%. We found that for the final printed structure to exhibit structural integrity, it is necessary to print at loadings above this value. Future work will include microscopy of both printed and cast samples to observe the dispersion and alignment of the CNCs within the polymer matrix and mechanical testing to show the effect of the reinforcement.

Poster No. 17

### **Mechanistic study of Listeria antibodies binding onto Au Nanoparticles at different pH conditions**

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Gold Nanoparticles (AuNPs) have emerged as an ideal vessel for biosensor purposes due to their unique surface characteristics, optical properties, stability, and consistency. To utilize AuNPs as a sensing substrate for pathogen detection, effective and stable interactions must be developed with targeted functionalities to create a high-quality biosensor. For this purpose, antibodies are an ideal biomolecule for site-specific delivery to pathogen cells due to their increasing availability, quality, and specificity. There is a well-established method for covalently binding the antibodies to carboxyl functionalized Au NPs through carbodiimide crosslinkers targeting Lysine residues on the antibodies. This reaction is highly dependent on the surface conditions of the particles, and thus the wet chemistry conditions of the solution suspending the particles. Simultaneously, the solution conditions greatly affect the stability and morphology of the particles, as well as the secondary structure stability of the antibody. In this work, we determine the balance between efficiency and stability of binding antibody as a function of pH and buffer solutions to carboxyl functionalized AuNPs using Listeria

monocytogenes targeting Antibodies. Overall, this work demonstrates aggregation, stabilization and binding mechanisms of *Listeria monocytogenes* antibodies onto carboxyl functionalized AuNPs at different pH conditions.

Poster No. 18

### **Host-Guest Nonlinear Optics using Amorphous Steroidal Lipids as Long Lifetime Host Materials**

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Research efforts in our group focus on the development of materials that exhibit nonlinear optical behavior. A 2013 study demonstrated the use of a steroidal lipid,  $\beta$ -estradiol, as a host material with nonlinear absorption.<sup>1</sup> With an observed lifetime on the order of 100 seconds, steroidal host materials provide the necessary environment for long triplet-state emission lifetimes. The study presented here demonstrates the application of a new steroid, lithocholic acid, along with  $\beta$ -estradiol and cholesterol, to long lifetime nonlinear optical materials. These glasses have been shown to minimize oxygen diffusion in steroidal materials and reduce nonradiative decay from excited states, thus extending the effective phosphorescence lifetime. While generation of long lifetimes using  $\beta$ -estradiol has been a main focus in the literature, the dangers of working with  $\beta$ -estradiol beg the transition to a safer substitute. Lithocholic acid, a naturally occurring bile acid, is shown here to be a satisfactory candidate for host-guest nonlinear optics moving forward.

Poster No. 19

### **Implication of nutrient concentrations related to a harmful algae bloom (HAB) and microcystin formation in Caesar Creek Lake, Wilmington, Ohio**

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Agricultural runoff poses a threat to the Wilmington, Ohio municipal water supply and its source waters. A harmful algae bloom (HAB) was documented in June 2017 near the intake site in Caesar Creek Lake. This study seeks to establish baseline nutrient concentrations in Caesar Creek Lake (Warren County, Ohio) and its tributaries, and to identify potential non-point sources of excess nitrogen and phosphorous. In collaboration with the Wilmington Water Department, dissolved inorganic nitrogen [DIN] (sum of  $\text{NH}_3$ ,  $\text{NH}_4^+$ ,  $\text{NO}_2^-$ ,  $\text{NO}_3^-$  concentrations), dissolved phosphorous [DP], particulate phosphorous [PP], total phosphorous [P]total (sum of [DP] and [PP] concentrations) and general water quality parameters were measured from May 30th, 2018 to the present in Caesar Creek Lake. General water quality parameters, [DP] and [DIN] samples were taken at depths of 0, 2, 6, and 11 meters. Microcystin samples were obtained and analyzed concurrently by the Wilmington Water Department. Ion chromatography was used to determine nitrite, nitrate, and phosphate in water samples. Sediment samples were obtained from tributaries to Caesar Creek Lake and were analyzed for both [P]total, [DP], and [PP] using inductively coupled plasma-optical emission spectrometry at 213.6 nm following acid digestion. A YSI Professional Plus electrochemical probe was used to measure general water quality parameters (E. coli, dissolved oxygen, pH, temperature, specific conductance). [DIN] ranged from 87.42

– 542.70  $\mu\text{M}$  from May 30th to July 11th, which was accompanied by an increase in microcystin (0.086 – 0.163  $\mu\text{g/L}$ ) during the same time period at 11 meters depth.

Undergraduate Researchers

Poster No. 20

### **Development of a Redox Active Metal-Tetrathiafulvalene catalyst**

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Tetrathiafulvalene (TTF) compounds exhibit great redox activity and characteristics via multiple, reversible redox reactions. The goal of this work is to create a versatile synthetic pathway to make TTF compounds for multiple applications. The successful synthesis of these precursors to the redox-active ligand will be achieved. Future work seeks to bind this ligand to a metal and test the catalytic properties of the metal-ligand complex

Poster No. 21

### **Cobalt Bis(dithiolene) N-Heterocyclic Carbene Adducts for Electrocatalytic Proton Reduction**

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Transition metal dithiolene complexes are unsaturated bidentate sulfur donor complexes have a variety of potential applications due to their stability and electronic properties. In recent years, research toward new catalyst developments has focused on develop electrocatalysts for proton reduction. Cobalt-bis(dithiolene) complexes demonstrated to be a robust system with promising activity on hydrogen production by electrocatalytic proton reduction. Here we report the synthesis, characterization and electrocatalytic proton reduction of four cobalt bis(dithiolene) N-heterocyclic carbene adducts. These complexes display considerable proton reduction activity under acidic condition.

Poster No. 22

### **Synthesis and Mechanistic Determination for Di(ferrocenylmethyl)imidazole-2-ylidene)-gold(I) and 1-mesityl(3-ferrocenylmethyl)imidazole-2-ylidene)-gold(I)**

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Gold(I) based compounds are known to inhibit thioredoxin reductase (TrxR) by targeting the thiol functional groups found within the Trx system. Our group previously synthesized and tested [Bis-(1,3-di(ferrocenylmethyl)imidazole-2-ylidene)-gold(I)] [chloride]. Cells treated with this compound increased reactive oxygen species by 14-fold compared to the control cells. These results indicate that ferrocenylated-gold(I) complexes are effective in killing cancer cells, but the mechanism is desired to be understood. The key concern in ascertaining the mechanism is whether the oxidation occurs at the ferrocene unit or at a different part of the molecule. To determine if the oxidation occurs at the ferrocene unit, 1-mesityl(3-ferrocenylmethyl)imidazole-2-ylidene)-gold(I) and di(ferrocenylmethyl)imidazole-2-ylidene)-gold(I)] [tetrafluoroborate] will be synthesized and then oxidized to determine the mechanism.

Poster No. 23

### **A Relaxation Kinetics Study of the Gas Phase Oxidation of Nitric Oxide**

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Nitric oxide is one of few “stable” molecules that may undergo termolecular elementary gas phase reactions with oxygen and with halogens. Such reactions are included in kinetic models of atmospheric chemistry. Despite a long history of experimental measurements of the rate coefficient for the gas phase oxidation of nitric oxide by oxygen,  $2 \text{ NO} + \text{O}_2 \rightleftharpoons 2 \text{ NO}_2$ , two expert panels, drawing from the same set of experimental results, have recommended rate coefficient values differing by a factor of two for use in atmospheric modeling. Further, it has been stated (Olbregts, 1985) that the  $\text{NO}_2$  product must be monitored directly in any kinetic study of this reaction because of its dimerization equilibrium with  $\text{N}_2\text{O}_4$ . In this research, the relaxation kinetics method has been applied for the first time to the oxidation of nitric oxide, and the  $\text{NO}_2$  dimerization equilibrium was incorporated into the integrated rate law, allowing for determination of the rate coefficient through total pressure measurements alone. This approach has proven to be successful, and a preliminary value,  $k = 2.3(3) \times 10^{-5} \text{ torr}^{-2}\text{-s}^{-1}$ , has been determined for the NO oxidation rate coefficient at 295(1) K. In addition to supporting the current NIST recommended rate coefficient value, this experimental method has potential applications in undergraduate teaching laboratories to demonstrate kinetics and equilibrium concepts.

Poster No. 24

### **The Role of Chromophore Isomerization in Laser-Induced Purple to Blue Transition in Bacteriorhodopsin**

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Bacteriorhodopsin is a trans-membrane protein found in the purple membrane of *Halobacterium salinarium*. It is formed of seven alpha helical coils arranged in a cylindrical fashion, with an organic molecule in the center of the protein. This chromophore is retinal, and it is this molecule that gives the purple membrane its color when it is bonded in the center of the protein. When a bacteriorhodopsin (BR) protein is irradiated with high-intensity light, and two photons of that light hit the BR, it causes the protein to go through a photocycle, or through a series of intermediates that end up back at the original BR. During this process, there is a conformational change in the molecule of retinal around a particular double bond.

The overall goal of this project was to identify the intermediate in the biphotonic bacteriorhodopsin photocycle where the second photon of light is absorbed. This would be identified using information known about the isomerization state of the retinal chromophore. Since the stage in the photocycle where this absorption occurs has been narrowed down to two places, and the two possible intermediates that could absorb the second photon have different chromophore conformations, locking the chromophore into one conformation could help identify which intermediate is the correct one. This could lead to an increased understanding of the bacteriorhodopsin photocycle, and because of the bacteriorhodopsin's similarities to rhodopsin, could lead to improved understanding of how light damages the human retina.

Poster No. 25

### **Molecular Dynamics Simulation Methods and Nuclear Quantum Effects**

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In this work, a B form fragment of single stranded DNA containing two bases of Thymine (dTpdT) was analyzed by observing the impact of nuclear quantum effects (NQE). Using molecular dynamics simulations methods, dimer formation and base stacking were observed by the addition of NQEs. Our approach involves calculating this influence using the ring polymer molecular dynamics method and comparing this to simulations without their inclusion. Results suggest that the base stacking of the thymine dinucleotide conformer behaves dissimilar to previous studies. The integration of nuclear quantum effects on dTpdT leads to reduced base stacking than otherwise found in previous simulations. Although more computationally expensive, it is suggested that NQEs be incorporated in future simulations.

Poster No. 26

### **Glyphosate Concentrations and a Measure of their Decay**

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Glyphosate is the weed killing chemical in Roundup, one of the most commonly used weedkillers in the world. Glyphosate was ruled carcinogenic in the part per trillion range to individual cells. It was also previously known to be extremely harmful to amphibians, causing major birth defects in the specimens it does not kill outright at concentrations of 3.7 ppm. Glyphosate concentrations and their decay rates were tested in both a bottled and an aquarium setting via gas chromatography-mass spectrometry following a derivatization method. Using this method it was found that storing Roundup in a cold and dark environment slows the decay of the glyphosate by 42% on a weekly basis. It was also found that glyphosate in an aquarium setting loses roughly a third of its concentration every week.

Poster No. 27

### **Dual-Stimuli Responsive Hyperbranched Polyamines For Gene Delivery Applications.**

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This project focuses on the use of stimuli-responsive, or “smart,” polymers as non-viral gene delivery vectors for gene therapy applications. The objective is to improve the transfection efficiency of a synthetic polycation, hyperbranched poly(ethylenimine), HPEI, by tailoring its solubility properties. A complex called a polyplex is generated through interactions of cationic HPEI and anionic DNA. HPEI is completely soluble in water, however, the addition of hydrophobic units leads to the observation of a lower critical solution temperature (LCST), which can be tuned by the choice of hydrophobic units added. The pH can also affect the LCST, which might be exploited to assist the HPEI to release its corresponding DNA payload. Introducing various ratios of groups such as isobutyramide, hydroxyl ethyl, butyl, hexyl, octyl, and dodecyl can lead to a finely tuned LCST. As such, a

series of modified HPEI systems have been prepared, and their pH dependent LCST behavior has been studied. Future work includes examining the transfection efficiency, adding a targeting agent for specific cell types and, finally, incorporating a blue fluorescent chromophore to track movements of the vector.

Poster No. 28

### **Bio-Templated Energetic Materials**

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Thermite reactions with nano-scale particles have been proven to have high combustion velocities and flame temperatures. Recently, hemozoin, a polymer of heme, can be combined with nano-aluminum particles (nAl) to generate larger energy outputs and higher combustion rates when compared to other nanocomposites (Naik, R et al Small. 2015, 3539). Hemozoin is naturally produced from heme by Plasmodium falciparum, the causative agent of malaria. Histidine rich proteins (HRPs) coordinate the crystallization of heme into a nontoxic and stable crystal using metal coordinating histidine repeats. We hypothesize that identification and optimization of protein sequences similar to HRPs will lead to efficient catalysts for hemozoin production. Here, we demonstrate the capability of Nvjp1 to produce hemozoin crystals. Nereis virens jaw protein 1 (Nvjp1) contains similar histidine motifs that can nucleate hemozoin formation. The iron-containing heme molecule incubates with recombinantly produced Nvjp1 to produce hemozoin as confirmed by FTIR. We then compared the hemozoin formation efficiencies of HRP and Nvjp1 proteins and compared the crystal morphologies by SEM imaging. The results show that Nvjp1 can facilitate hemozoin formation which expands the range of possible proteins that will template heme crystallization. The future directions of this project will attempt to modulate the shape and size of the hemozoin crystals to increase the possible energy output of thermite nanocomposites.

Poster No. 29

### **The Effect of Polymer Geometry on its Miscibility with 1,8-Diiodooctane: A Computational Study of the Polymer:Fullerene Bulk Heterojunction**

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The use of multicomponent materials has played a critical role in enhancing the performance of polymer-based devices, including organic photovoltaics and other various sensors. With such materials, miscibility becomes important, and understanding how to control film morphology with the use of various solvents and solvent additives has attracted considerable interest as a path towards influencing device efficiency. This work focuses on using molecular simulations to determine the miscibility of the solvent additive DIO with fullerene-derived molecules, PC61BM and PC71BM, and variable length oligomers of P3HT and PTB7. Specifically, the interaction parameter  $\chi$ , defined within the Extended Flory- Huggins Theory (EHFT), was obtained from the simulations. Energy minimization at 298.15 K was initially performed for all structures. The COMPASS forcefield successfully modeled the structures. P3HT resulted to be periplanar with torsion angles of  $0^\circ$  to  $0.75^\circ$ , and PTB7 was predicted to have a helical coil geometry. Values of  $\chi$  between DIO and PC61BM/ PC71BM were determined to be 24.3 and 21.7, respectively. For DIO with P3HT,  $\chi$  was determined to increase linearly with increasing n, and for DIO with PTB7,  $\chi$  was determined to increase linearly up to  $n = 10$ . We find that DIO is more miscible with the fullerenes than with the oligomers with as small as ten units, thus supporting the preferential mixing of

DIO with fullerenes as observed in experimental investigations, where even much higher molecular weight polymer chains ( $n \gg 10$ ) are used.

Poster No. 30

### **Photophysical Impact of Varying Amine-Donor Substitution Position in a Series of Naphthalenecarbonitriles**

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Controlling ground- and excited-state properties of organic chromophores is important in many areas such as photovoltaics, biological sensors, display technologies, and photochemical synthesis, to name only a few. Our group has historically been interested in how to control the nonlinear properties of chromophores, in particular, the excited-state absorption (ESA). Tuning the oscillator strength, breadth, and energy of the ESA allows for control of the nonlinear performance. However, examples of how to tune ESA are sparse. In this work, a group of naphthalenecarbonitrile derivatives containing electron donating groups (either dimethylamino or piperidiny) in the 2-, 3-, or 4- positions are synthesized. The changes in substitution position dramatically affect the energy of the ESA transitions, with shifts in the maxima greater than 100 nm. These modifications also impact the singlet state, as fluorescence lifetimes and quantum yields are significantly larger in the 3-substituted compounds than the 4-substituted. Another significant effect of varying the substitution positions is the singlet-triplet energy gap, which can be tuned from 0.65 eV (2-position) to 1.01 eV (4-position).

Poster No. 31

### **Development and Investigation of Antibiotic Resistance Models in E. coli Using Aminoglycosides and Beta-lactams**

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The use of antibiotics to cure bacterial infections is one of the single most significant medical advancements in human history. This research focuses on the ability of bacteria to develop resistance to these antibiotics. The aminoglycoside antibiotic kanamycin and the beta-lactam ampicillin were used to develop resistance in E. coli (ATCC 25922) as high above the minimum inhibitory concentration (MIC) as possible. Resistance was developed up to 2500  $\mu\text{g}/\text{mL}$  of kanamycin, 100 times the MIC of 25  $\mu\text{g}/\text{mL}$ . With ampicillin, resistance was propagated up to 200  $\mu\text{g}/\text{mL}$ , 50 times higher than the 4  $\mu\text{g}/\text{mL}$  MIC found in literature. The antibacterial-resistant E. coli were then used in a cross-resistance study. This study aimed to find whether kanamycin resistance or ampicillin resistance translated to resistance to other antibiotics. The kanamycin-resistant E. coli were tested against neomycin and gentamicin (both aminoglycosides) and ampicillin (a beta-lactam). The kanamycin-resistance did not confer resistance to ampicillin, but resistance above the wild-type MIC was seen with gentamicin and to a larger extent with neomycin. Conversely, ampicillin-resistant strains had slightly elevated resistance to kanamycin.

# Acknowledgment of Judges

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SAMPE Midwest Chapter and ACS Dayton Section would like to thank the following volunteers for contributing their time and expertise to judge the posters. This is a very high number of judges for each event.

## SAMPE Midwest Chapter Student Research Symposium

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