



Annual Poster Session  
and  
Patterson College Chemistry  
Awards Ceremony

April 4<sup>th</sup>, 2018 (Wednesday)

5:30 – 8:00 pm

Ballroom, John F. Kennedy Memorial Union,  
University of Dayton

# Welcome

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Welcome to the annual poster session of the Dayton Section of the American Chemical Society! In this event, we will share and celebrate the research achievements of researchers at all levels – but particularly those of graduate and undergraduate students – in the area.

In addition to this, thanks to the generous bequest of the Patterson family, we are able to award the best junior Chemistry majors in each of the schools in the area the *Patterson College Chemistry Award*. We look forward to celebrating their achievements as well.

We look forward to meeting all of you and hope you will have a good time at this event! To know more about the Dayton Section, please go to our website at <http://daytonacs.org/> or visit us on Facebook (<https://www.facebook.com/daytonacs/>).

## Agenda

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5:00 – 5:30 pm: Poster Set-Up

5:30 – 7:30 pm: Poster Session and Student Poster Judging

7:30 – 8:00 pm: Award Presentation

## Officers of the Dayton Section

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Chair:	Dr. Anastasie Weaver
Chair-Elect:	Dr. Erick Vasquez
Immediate Past Chair:	Dr. Eugeniya Iskrenova-Ekiert
Treasurer:	Dr. Prakriti Pollack
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.

## About The Section

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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 450, covering the counties of Montgomery, Greene, Miami, Clarke, 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**, and contributes funds and judges for the **West District Science Fair**

## About the Host Institution

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The Poster Session is held at a different university in the Dayton area each year. This year, we are pleased to be holding this at the University of Dayton.

The University of Dayton, affiliated with the Marianist order of the Catholic Church since its founding in 1850, Chemistry has been taught at 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 and 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 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 thanks Provost Paul Benson, Dean of the College of Arts and Sciences Jason Pierce, Chemistry Department Chair David Johnson, and the School of Engineering as well as all the department faculty and students of the University of Dayton for welcoming, hosting, and providing support for the 2018 ACS Poster Session.

# 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:

- Joseph Zavodney, Cedarville University
- Arame A. Diouf, Central State University
- Joshua Killian, University of Dayton
- Bradley Mallott, Wittenberg University
- Jeremiah Stevens, Wright State University

The Dayton Section of the American Chemical Society offers its sincere congratulations to the awardees. A brief biography of each of the awardees follows:

## Joseph Zavodney, Cedarville University

Joseph Zavodney is a junior B.S. Chemistry student at Cedarville University. He has been involved in the chemistry club, and is currently doing research with Dr. Sekerak in the field of polymer chemistry. Joseph has a large amount of lab experience having taken most of the required courses for the major and even passed his thermodynamics and kinetics class. Joseph is also involved in various extracurricular activities. He is a residence assistant over 20 fellow students and leads them in community development, spiritual vitality, and personal growth. Joseph has been the social coordinator for an organization on campus and will continue in that role for the following academic year. This organization has surrounded Joseph with men who push him toward spiritual growth and this has been a large area for character growth in his life. He has been a tutor employed by the Academic Enrichment Center. Outside of the University, Joseph is very involved in a local church to continue to develop his character. Joseph continuing to strive for academic excellence and pursues holiness in his disciplines. This award means much to Joseph and he is honored to accept it and is spurred on by this nomination to continue to pursue faithfulness in academics and in character development. His future plans are not set in stone but further education in graduate school is an interest as well as working as a chemistry teacher or working in a lab after graduation. Joseph is interested in inorganic research or analytical lab work and would most likely pursue one of these avenues in the near future.

## Arame A. Diouf, Central State University

Arame A. Diouf was born in Dakar, Senegal on 12 July 1998. She is the oldest of five children and she attended The Senegalese American Bilingual School in her home country. There, she was in the Senegalese education system which is based on its French equivalent for most of her high school curriculum. She transferred into the American program where she took her 11<sup>th</sup> and 12<sup>th</sup> grade classes. Her interest in Chemistry was largely influenced by her high school Chemistry teacher who challenged her. Arame graduated as the valedictorian of her class.

Arame enrolled at Central State University (CSU) in the fall of 2015. She has an interest in medicine and her professional goal is to become an anesthesiologist. Therefore, she is majoring in Chemistry. While at CSU, Arame is involved with the Honors program and has been the top scholar for her freshman, sophomore, and junior class. She works as a Resident Assistant and a tutor assisting her residents and fellow classmates in

chemistry, math, biology and French. She also founded the International Student Association and had the opportunity to serve as the Vice-President of the Minority Association of Pre-Med Students. During the summer of 2017, Arame interned at The University of Akron where she worked on synthesizing single chain polymer nanoparticles for carbon dioxide capture. She also does undergraduate research under her chemistry teacher Dr. Katampe conducting experiments for the synthesis of bioactive polymers from natural sources.

## Joshua Killian, University of Dayton

Josh Killian is a junior Chemistry major at the University of Dayton. He was born and raised in Pittsburgh, Pennsylvania and is an avid Pittsburgh sports and Tottenham Hotspur soccer fan. Josh is a Resident Assistant and is involved in several organizations at UD. He plays trumpet in the Flyer Pep Band, participates in a variety of intramural sports, and is a student leader in a campus ministry organization, The Navigators. This summer, Josh will be participating in research led by Dr. Vladimir Benin here at UD regarding [2+2] cycloadditions of newly synthesized azophosphonates and azobisphosphonates with ketenes. After graduation, Josh plans to either pursue a PhD in the field of chemistry or teach and coach at the high school level.

## Bradley Mallott, Wittenberg University

Bradley Mallott was born and raised in Middletown, Ohio and attended Madison Local Schools from kindergarten through 12th grade. He is a pre-med student and is working towards a B.A. in chemistry. Brad was a two-year starter on the Wittenberg baseball team and is the President-elect of the chemistry club. He also enjoys playing basketball and tennis and listening to music in his free time.

Brad has been exposed to science from young age as his mother, Cindy, is a chemistry and physics teacher at Madison High School and he took a special interest in chemistry during high school. Brad has earned a 3.9 GPA at Wittenberg and is a member of the Phi Eta Sigma honor society. He hopes to attend medical school in the fall of 2019.

Throughout his time at Wittenberg, Brad has volunteered at the Rocking Horse Community Health Center in Springfield, Ohio and completed a clinical internship at Comprehensive Eye Care under Molly O'Neill, O.D. This summer, Brad has the privilege to work with Dr. Daniel Marous at Wittenberg University on research of antibiotic resistance among bacteria.

## Jeremiah Stevens, Wright State University

Jeremiah Stevens is a chemistry undergraduate student at Wright State. He graduated from Beaver Creek High School and immediately after enrolled at Wright State. After graduating from Wright State with his B.S. in chemistry in Spring 2019, he intends to pursue a Ph.D. in physical chemistry (likely at The Ohio State University) in order to become a professor.

Teaching and chemistry are his two largest passions in life, so teaching chemistry as a career would be his dream come true. He started tutoring chemistry when he was still in high school, but he was given opportunities to serve in more formal teaching roles once he got to Wright State. He started in Spring 2017 as a learning assistant in General Chemistry II before becoming a teaching assistant in Fall 2017. As a teaching assistant, he has taught General Chemistry I labs and even a few General Chemistry II pre-lab recitation sections, and he has loved every last second of it. In his remaining time at Wright State, he hopes to continue teaching, but he will also be working on nanocomposite materials research with Dr. Rachel Aga. He will start

this summer, and he is incredibly excited to be joining Dr. Aga's team! In addition to being a student at Wright State, he is also a member of the American Chemical Society and the American Mensa.

Chemistry runs through his veins, and he especially loves physical chemistry. There is a certain *je ne sais quoi* about p-chem that just really piques his interest. He loves learning about the intricacies of chemistry, and the level of detail that p-chem provides is absolutely amazing to him. He has a voracious appetite for knowledge, and the many facets to p-chem provides ample opportunities for him to learn new things. In fact, his primary hobby is learning chemistry. He has quite a vast collection of chemistry textbooks, and he often reads them in my spare time. When he need to relax, he usually picks a chemistry textbook off my shelves and do some of the exercises in it.

Jeremiah would like to thank all of the Wright State Chemistry Department faculty for all that they do. He would like to especially thank Dr. Rachel Aga, Dr. David Dolson, Dr. Steven Higgins, Dr. Eric Fossum, Dr. Daniel Ketcha, Dr. Kuppuswamy Arumugam, Mr. Jonathan Grieb, Dr. Lary Sanders, Dr. Travis Clark, and Mr. Garrett VanNess for sharing their knowledge, experiences, and enthusiasm for chemistry with me in the classes I had with them thus far. He regards myself as very lucky to have the opportunity to learn from such a diverse, talented, and amazing group of faculty members, and will be eternally grateful for all that they have done for him.

# Poster Session Abstracts

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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

### **A QM/MM equation-of-motion coupled-cluster approach for predicting semiconductor color-center structure and emission frequencies**

Lutz, J. J.\*; Duan, X. F., Burggraf L. W.

*Department of Engineering Physics, Air Force Institute of Technology*

Valence excitation spectra were computed for deep-center silicon-vacancy defects in 3C, 4H, and 6H silicon carbide (SiC) and comparisons were made with literature photoluminescence measurements. Optimizations of nuclear geometries surrounding the defect centers were performed within a Gaussian basis-set framework using many-body perturbation theory or density functional theory (DFT) methods, with computational expenses minimized by a QM/MM technique called SIMOMM. Vertical excitation energies were subsequently obtained by applying excitation-energy, electron-attached, and ionized equation-of-motion coupled-cluster (EOMCC) methods, where appropriate, to small models including only a few atoms adjacent to the defect center. We consider the relative quality of various EOMCC and time-dependent DFT methods for (i) energy-ordering potential ground states differing incrementally in charge and multiplicity, (ii) accurately reproducing experimentally measured photoluminescence peaks, and (iii) energy-ordering defects of different types occurring within a given polytype. The extensibility of this approach to transition-metal defects is also tested by applying it to silicon-substituted chromium defects in SiC and comparing with measurements. It is demonstrated that, when used in conjunction with SIMOMM-optimized geometries, EOMCC-based methods can provide a reliable prediction of the ground-state charge and multiplicity, while also giving a quantitative description of the photoluminescence spectra, accurate to within 0.1 eV of measurement for all cases considered.

Poster No. 2

**Thermal Behavior of Gold Nanorods in a Structural Polymer Matrix**

Izor, S.\* , Kennedy, W. J., Varshney, V., Anderson, B., Koerner, H., Ehlert, G. J.

*Materials and Manufacturing Directorate, Air Force Research Laboratory; UES Inc.; Universal Technology Corporation*

Understanding the fundamental mechanisms that govern gold nanorod shape transformation opens up possibilities for a variety of sensing applications. In this work, we investigate the time-resolved thermal reshaping for gold nanorods of different geometries (aspect ratio, volume) in a crosslinked epoxy matrix at application-relevant temperatures (120°-220°C). Our analysis suggests that the initial particle geometry largely impacts the ultimate extent of reshaping at a given temperature. In addition, the observed nanorod reshaping dynamics can be divided into two temporal regimes that are controlled by different phenomena. At short times, shape transformation is dominated by a curvature-induced surface diffusion process in which the activation energy for diffusion depends on particle geometry. At long times, external forces from the surrounding environment impede diffusion and stabilize the nanorod shape.

Poster No. 3

**Insights into the ligand induced distortion of molecular geometry in N-heterocyclic carbene Iron-bis(dithiolene) adducts**

Selvakumar Jayaraman and Kuppuswamy Arumugam\*

*Wright State University*

Our efforts are directed towards understanding the molecular geometry of iron-bis(dithiolene) N-heterocyclic carbene adducts. We predict that NHC ligands induce distortion from a square pyramidal molecular geometry to trigonal bipyramidal geometry. This poster describes a systematic study of this geometry deviation in iron-bis(dithiolene) N-heterocyclic carbene adducts. The ambiguity behind molecular structure deviation was analyzed with the guidance of steric and electronic factors gleaned from theoretical and X-ray structural analysis.

## Graduate Students

Poster No. 4

### **Initial Study of Novel Flame Retardants For Epoxy Resin Systems**

Bin Sulayman, Abdulhamid\*; Klosterman, Donald; Benin, Vladimir; Morgan, Alexander  
*Chemical and Material Engineering department; Chemistry department; University of Dayton*

This poster describes the initial investigation of the reaction between a novel flame retardant (FR) and epoxy resin. The novel chemical (synthesized and provided by UD Chemistry Department faculty) is a phosphorous based flame retardant that also incorporates primary and/or secondary amine functional groups. These groups potentially could react with epoxy resins, which would then incorporate this FR chemical directly into the polymer network through covalent bonding. This would be a way of introducing flame retardants into epoxy resins to improve flammability of composites. Initial research was conducted using Differential Scanning Calorimetry (DSC), Thermogravimetric Analysis (TGA), and Fourier Transform Infrared Spectroscopy (FTIR). The results indicate that the flame retardant is indeed reacting with the epoxy resin to form a crosslinked network. Future work will involve characterization of the cured epoxy-FR network for physical properties, mechanical properties, and flammability.

Poster No. 5

### **Synthesis and Characterization of Silane and Siloxane Phthalonitrile Polymers**

Monzel, W. J. \*(a); Lu, G. Q. (a); Pruyn, T. L. (c); Houser, C. L. (b); Yee, G.T. (b)  
*(a) Department of Materials Science and Engineering, Virginia Tech (b) Department of Chemistry, Virginia Tech (c) Polymer Matrix Composites Group, Air Force Research Laboratory*

Polymers from phthalonitrile-containing monomers are of interest for high temperature applications. It is desirable to improve their processing and thermo-oxidative stability. With optimum thermal stability in mind, phthalonitriles with carbosilane and carbosiloxane linkages were synthesized in high yields. The monomers possessed relatively high melting points, but no hydrolytic sensitivity was observed. Desired processing characteristics were achieved with 4-6 wt.% of an amine catalyst. Materials were cured to 350-375°C. The carbosilane-phthalonitrile polymer exhibited glass transitions above 290 °C. The Tg of the carbosiloxane-phthalonitrile was limited to 170-200°C. High coefficients of thermal expansion were observed for silicon containing resins. Post-curing for additional time at 350-375°C increased the Tg and decreased the CTE of the carbosilane-PN but not the carbosiloxane-PN. Both polymers showed excellent stability in TGA. When aged in air at 250°C, these materials showed higher weight and volume loss compared to commercial organic phthalonitrile resins.

Poster No. 6

### **Thermal Engineering of Flexible, High-Power Electronics**

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

<sup>1</sup>*Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, 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, Wright-Patterson Air Force Base, OH 45433 USA*

Consumers and military personnel are demanding faster data speeds only available through fifth generation (5G) wireless communication technology. The challenge is to enable electronic devices to withstand strain and continue to operate within an acceptable tolerance to ensure reliability. A fundamental challenge for flexible electronics is thermal management. Even on rigid substrates with higher thermal conductivity than flexible substrates, the full potential of semiconducting materials is often thermally limited. The flexible gallium nitride (GaN) transistors employed in this work are grown on a two-dimensional boron nitride release layer that allows the conventionally processed devices on sapphire wafers to be transferred using a polymeric stamp and placed onto a variety of rigid and flexible substrates. Characterization of the GaN device behavior on the as-grown sapphire wafers (not transferred) provide a baseline for evaluation of the thermal performance. Transferring the GaN devices to flexible substrates enables application of strain during device operation; however, device performance typically suffers due to the low thermal conductivity of most polymeric substrates. In situ thermal imaging of devices in operation reveals that the current passing through a non-transferred GaN transistor on a sapphire wafer reaches the target operating temperature at twice the current of the same device transferred to a flexible substrate. Packaging environment simulations and consideration of device-substrate interfacial thermal effects allow for an understanding of how the flexible GaN devices operate after they are transferred to a substrate and show the path forward for substrate design to reduce thermal limitation of high-power flexible electronics.

Poster No. 7

### **Discovering inhibitors of bacterial efflux pumps**

Auer, Erich\*; Lopper, Matthew E.

*University of Dayton Department of Chemistry*

Overuse of antibiotics has contributed significantly to the emergence of antibiotic resistance in bacteria. As bacteria adapt to antibiotics, current treatments become ineffective and bacterial infections can become life threatening. While bacteria can develop resistance to antibiotics in many different ways, one of the mechanisms that can confer resistance to multiple classes of antibiotics is the overexpression of efflux pumps. Efflux pumps are membrane transporters that are capable of taking potentially harmful substances, like antibiotics, from inside the bacterial cell and moving them out. This allows the bacterium to escape from the killing effects of the antibiotics. Here, we employed high-throughput virtual screening and a fluorescence-based efflux assay to identify compounds that could bind to and inhibit the activity of the *E. coli* AcrA-AcrB-TolC efflux pump. Of the many sites on AcrB and TolC that we targeted in our docking studies, only one site in the interior of AcrB proved to be productive for finding inhibitors of efflux pump activity.

Poster No. 8

**Development of a Redox Active Switchable Catalyst Containing Tetrathiafulvalene**

Miles, M.\*; Jarnagin, C.; Arumugam, K.  
*Wright State University Chemistry Department*

Tetrathiafulvalene (TTF) is a stable redox active molecule capable of undergoing multiple one electron reversible redox transformations. This unique characteristic coupled with the catalytic nature of an N-heterocyclic carbene (NHC) metal complex makes it possible to synthesize a redox-active catalyst capable of “switching” the metal’s selectivity towards a variety of substrates. NHCs have proven to be very successful catalysts due to their tunable properties, stability, and electron donating properties. By changing the oxidation state of TTF, the stable NHC catalyst can access three or more catalytic species. Hence, the synthesis of a TTF-NHC-Iridium complex is currently being explored. Structurally, the complex will be analyzed by Nuclear Magnetic Resonance Spectroscopy (NMR) and single crystal X-ray diffraction crystallography. Various electrochemical tests will also be employed to test the complex’s redox properties.

Poster No. 9

**Redox-active Silver N-Heterocyclic Carbene Complexes: A Dual Targeting Anti-bacterial Drug**

Malek, Kotiba\*; Metzger, Jared; Arumugam, Kuppuswamy  
*Wright State University*

Bacterial resistance to current antibiotics necessitates new therapeutic approaches. Silver-based drugs offer a promising alternative due to their antibacterial properties. Recently, N-heterocyclic carbenes (NHC) containing silver complexes have become a popular subject of research due to their versatility and stability. To further enhance the efficacy of silver NHC complexes as antibacterial agents, redox-active ferrocenes were introduced in this study. Ferrocenes have shown to increase reactive oxygen species (ROS) production, which results in cell death. Six new potential antibacterial silver-NHC complexes with redox activity were synthesized and confirmed via analytical techniques, including  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy.

Poster No. 10

**Aerosol Jet Printing of SU-8 for Capacitor Applications**

Richard A Williams III<sup>a</sup>, and Rachel S. Aga\*  
*Department of Chemistry, Wright State University, Dayton, OH 45435, USA*

As the demand for smaller devices is increasing, better fabrication methods are needed for new and existing materials. The development of direct writing and additive manufacturing technology have allowed for the continued miniaturization of devices, and this technology has not yet been explored to its full potential. In this study, an aerosol jet fabrication process of the polymer material SU-8, for capacitor applications is investigated. Aerosol jet printing is a direct writing and additive manufacturing technique that allows for control over the deposition pattern and thickness. Through variation of printing parameters and the film curing process, the effect of each parameter on thickness and dielectric properties of the film can be determined. A trend is seen between the post exposure bake and the dielectric constant of the resulting devices. In addition, printed devices have been observed to have a higher dielectric constant than devices fabricated by spin coating.

## Undergraduate Students

Poster No. 11

### **Engineered Microbe to Sense and Respond to Travelers' Stomach**

Bete, A.; Carter, J.; Davis, C.\*; Dong, J.; Herrmann, M.; Jesse, H.; McDonald, D.; Menart, P.; Poole, A.\*; Smith, A.

*Carroll High School, Air Force Research Laboratories, UES Inc., Wright State University - Biochemistry and Molecular Biology Department*

Every year, Enterotoxigenic Escherichia coli (ETEC), the most common form of traveler's diarrhea, affects thousands of deployed personnel. The goal of this research is to engineer non-pathogenic E. coli to sense ETEC, respond to its presence, and package it in a cellulose matrix to enable environmental detection of ETEC. Two plasmids were created: 'sense-respond'; and 'packaging'. The sense-respond plasmid detected autoinducer 2 (AI-2), a quorum sensing molecule created by most ETEC strains, by expressing LsrR which switches on the Lsr promoter. Activation of the Lsr promoter expresses superfolder green fluorescent protein (sfGFP), indicating the presence of ETEC. The packaging plasmid expresses a fusion protein consisting of curli fibers and cellulose binding domains. These modified surface proteins permit the bacteria to bind to cellulose, encapsulating the sense-response module. This genetically engineered machine could be deployed in both the internal and external environment to detect ETEC.

Poster No. 12

**A Raman-Based Imaging Method for Characterizing the Molecular Adsorption and Spatial Distribution of Silver Nanoparticles on Hydrated Mineral Surfaces**

Brittle, S. W.; Foose, D. P.; O'Neil, K. A.; Sikon, J. M.\*; Johnson, J.K.; Stahler, A. C.; Ryan, J.; Higgins, S. R.; Sizemore, I. E.

*Wright State Department of Chemistry*

Silver nanoparticles (AgNPs) currently represent over 54% of the total number of consumer products containing nanomaterials, mostly exploiting their unique antimicrobial properties. However, little is known about AgNPs released into the environment through irrigation and rainfall and their interactions with one of the major components of soil (~45%), minerals. The main goal of this study was to develop a label-free or label-enhanced micro-Raman-based mapping method for imaging the distribution of AgNPs on various mineral surfaces and their potential molecular interaction mechanisms. This new methodology was successfully tested on a) two macro- and micro-sized mineral models, muscovite [ $KAl_2(AlSi_3O_{10})(OH)_2$ ] and corundum ( $\alpha-Al_2O_3$ ), and b) two positively and negatively charged AgNPs models, under key environmental conditions (ionic strength and pH). Collected Raman maps (n = 625-961 spectra each) were rapidly analyzed using well-established chemometric methods in Vespucci, a free open-source software developed by our group, and the Raman results were confirmed by ICP-OES, AFM, and SEM-EDX. Covalent interactions through the formation of Ag-O-Al- bonds were detected in a label-free manner for both AgNPs<sup>+</sup> and AgNPs<sup>-</sup>, when exposed to corundum minerals (pHpzc = 9.1), thereby potentially reducing the environmental mobility of these AgNPs. No molecular interactions were identified in between AgNPs<sup>-</sup> and muscovite in the label-free Raman approach; thus, label-free Raman imaging was developed for mapping the scarce spatial distribution of AgNPs<sup>-</sup> on such mineral surfaces. The proposed Raman-based imaging requires minimum to no sample preparation; is sensitive, noninvasive, cost-effective; and might be extended to other environmentally relevant systems or other metallic nanoparticles.

Poster No. 13

**Cobalt Bis(dithiolene) N-Heterocyclic Carbenes and their use as Electrocatalysts for Proton Reduction**

Leedy, C.\*; Jayaraman, S.; Arumugam, K.

*Wright State University Chemistry Department*

Cobalt-bis(dithiolene)-N-heterocyclic carbene adducts [ $Co(S_2C_2Ar_2)NHC$ ] with Phenyl and p-anisyl substituted on dithiolene fragments and 1,3-bis(mesityl)-imidazole (IMes) and 1,3-bis(mesityl)-imidazolium (SIMes) N-heterocyclic carbene were planned to be synthesized. After synthesis and characterization, all four adducts will be evaluated for electrochemical two electron reduction and concomitant N-heterocyclic carbene release from the adducts [ $Co(S_2C_2Ar_2)NHC$ ]. At present we have synthesized [ $Co(S_2C_2-p-anisyl)IMes$ ] and [ $Co(S_2C_2-phenol)IMes$ ]; synthesis of the other two complexes is under way.

Poster No. 14

**Mechanistic Determination for di(ferrocenylmethyl)imidazole-2-ylidene-gold(I)**

Evers Smith, Catherine\*; Jarnagin, Clark\*; Miles, Meredith; Arumugam, Kuppuswamy  
*Wright State University Chemistry Department and Wright State University*

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, di(ferrocenylmethyl)imidazole-2-ylidene-gold(I) [tetrafluoroborate] will be synthesized and then oxidized to determine the mechanism.

Poster No. 15

**The Impact of the 515nm Effect on Singlet Oxygen Quenching in Photosynthesis: Model System Studies Using  $\beta$ -Carotene–Acid Complexes**

Lauren A. Hoody, Caoqinglong Huang, Ashlee E. Wertz, Mark B. Masthay  
*University of Dayton Chemistry Department*

$\beta$ -carotene ( $\beta$ C) is an orange biological pigment present in green plants, where it plays a protective role against the potential harmful effects of light.  $\beta$ C does this by deactivating “singlet oxygen”, which is a toxic molecule generated during photosynthesis. During photosynthesis,  $\beta$ C temporarily converts from its native orange state to a pink state. We hypothesized that pink  $\beta$ C reacts with singlet oxygen less efficiently than native orange  $\beta$ C. To test this hypothesis, we chemically modeled  $\beta$ C’s pink state with blue  $\beta$ C–acid complexes, which are chemically similar to pink  $\beta$ C, created by reacting  $\beta$ C with trichloroacetic acid (TCA).  $\beta$ C’s efficiency at deactivating singlet oxygen was characterized by measuring the rate of degradation of 1,3-diphenylisobenzofuran (DPBF), which has a high reactivity towards singlet oxygen and is used to detect the amount of singlet oxygen in a solution. Our DPBF–based results to date indicate that native orange  $\beta$ C and blue  $\beta$ C–TCA complexes quench singlet oxygen with roughly equal efficiency. In the summer of 2018 we intend to confirm our DPBF–based results by monitoring the impact of  $\beta$ C and  $\beta$ C–TCA complexes on the 1270 nm (near–infrared) emission of singlet oxygen using a state–of–the–art, time–resolved near–infrared spectrometer.

Poster No. 16

### **Glyphosate Concentrations in River and Stream Water as a Function of Rain Runoff**

Snider, J.; Dudek, R

*Wittenberg Chemistry Department*

Glyphosate is the weed killing chemical in Roundup, one of the most commonly used weedkillers in the world. It is advertised as being able to kill weeds, but not the lawn or crops around the weeds. It is mostly used against broadleaf plants, halting their EPSP synthase and killing them within a week. After application, it will begin to decay microbially into aminomethylphosphonic acid (AMPA), and can possibly get into water sources via runoff as either glyphosate or as its decayed AMPA form. Glyphosate was ruled carcinogenic in the part per trillion range to individual cells on July 7, 2017, by the California Office of Environmental Health Hazard Assessment. 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<sup>2</sup>. A method for the analysis of stream and river water for traces of glyphosate and AMPA was established using Gas Chromatography-Mass Spectrometry following a derivatization process with fluorenylmethyloxycarbonyl chloride (FMOC-Cl). Samples of water for testing were collected from 5 sites in Clark County, OH, within 5 days of a rainfall.

Poster No. 17

### **UV Assisted Direct Ink Writing of Pre-ceramic Polymers**

Wyckoff, C.\*; Rueschhoff, L.; Dickerson, M.

*Wright State University, AFRL Materials and Manufacturing Directorate*

A new method of UV assisted direct ink write additive manufacturing (UV-DIW) of silicon nitride loaded pre-ceramic polymers is presented. UV exposure while printing allows for more complex structures and for a wider range of ceramic processing routes. Previous works use highly loaded aqueous solutions, UV-DIW of epoxies, or different additive manufacturing techniques. A previously established pre-ceramic polymer-based resin for stereolithography was modified by silicon nitride power loading and the addition of sintering aids. Ceramic green bodies were made with a 3D printer extruding the ink out of a syringe via displacement while being exposed to UV light. Fired parts exhibit a reduced amount of shrinkage, 4%.

Poster No. 18

### **Liquid Crystalline Polymer Networks Retaining the Blue Phase Over Wide Temperature Ranges**

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Blue Phase (BP) liquid crystals are of considerable scientific and technological interest for their photonic properties. BP liquid crystals offer optical anisotropy independent of viewing angle and can be created without the need for an alignment layer. These properties allow for the improved performance and simplified fabrication of liquid crystal based electronic optical devices. BP states typically have a temperature range of 1 Celsius degree, thus extension of the temperature range for BP liquid crystals is essential for their use in optical devices. Our group has extended the temperature range of the BP states via photopolymerization to form temperature stabilized polymer networks in the liquid crystal cells. BP mixtures were created using 62.2 wt% chiral monomer CM04151 and 37.8 wt% achiral mesogen ST05953 along with 1 wt% photoinitiator Irgacure-651. The mixture was placed inside a 20-micron polyimide coated cell and then placed in a heating stage at 120 °C under a polarized optical microscope. The mixture was slowly heated until phase change to BP and subsequently exposed to UV light to initiate photopolymerization. BP was observed in a temperature range of 116.5 °C – 115.3°C and stabilized polymer films maintained BP at room temperature. Future work includes additional characterization of the liquid crystal networks via Kossel diagramming to assure that we realized the blue phase and identify which variant. Using this project as a starting point, the group intends to explore the realization of a blue phase liquid crystal elastomer by using synthetic methods concurrently developed in the group

Poster No. 19

### **Localizing Strain in Patterned Liquid Crystal Elastomers**

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Liquid crystal elastomers uniquely exhibit anisotropic properties which are utilized in numerous applications such as flexible electronics and optical devices. The importance of the mesogen orientation greatly influences the mechanical behavior of these samples. In this project, we investigated the ability to localize strain in predetermined regions in multiple directions of stretch by using four types of mesogenic alignments: polydomain, homeotropic, twisted, and planar. In one case, we tested a sample containing both polydomain and homeotropic alignment. The strain was primarily localized in the homeotropic regions while the polydomain regions were significantly lower. This phenomenon is due to the omnidirectional soft elasticity observed in the homeotropic orientation leading to a lower modulus of elasticity than the polydomain. We are further extrapolating this data to analyze auxetic patterns and determine if it is possible to lower the Poisson's ratio in a liquid crystal elastomer.

### **Conformational Change of the Glucose/Galactose-Binding Protein**

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Galactose/glucose-binding protein (GGBP) is a periplasmic monomeric protein found in a number of gram negative bacteria, including *Escherichia coli* (Fonin, et al. 2017). The protein stimulates chemotaxis towards D-galactose and D-glucose and binds with a high affinity to glucose (Fonin, et al. 2017). GGBP is made up of two globular domains that are connected by a hinge region to form the sugar binding site (Borrok, et al. 2007). When the protein interacts with the ligand, it undergoes significant conformational changes (Brown, et al. 2016).

Understanding how the ligand binds with the protein and the free energy change associated with the protein conformational change is the focus of this research. GROMACS was used to perform free energy molecular dynamic simulations. Using center of mass pulling to move one of the globular domains of the protein in the closed form, GGBP was forced open while bound to the  $\beta$ -anomer of glucose. Umbrella sampling and Weighted Histogram Analysis Method (WHAM) were used to determine the free energy change of the system.