

**CONTROL ID:** 2210996

**CONTACT (NAME ONLY):** [Li Yao](#)

**TITLE:** [Calculation of the anharmonic effect of elementary reactions of high-temperature combustion reaction](#)

**ABSTRACT BODY:**

**Abstract:** Abstract

Combustion plays an important role in engineering and our life. Today, about 90 percent of the energy is generated by the combustion in our world [1]. Focusing on the chemistry of combustion of fuels, it is of great significance to design the combustion chamber, control pollutants and research on alternative fuels [3-4]. The chemical kinetic mechanism of combustion of fuels is composed of a series of elementary reactions. Therefore, to better grasp the mechanism of combustion reaction, it is necessary to investigate the elementary reaction process. Being the key parameters of the chemical kinetic mechanism of the combustion reactions, the rate constants are calculated using RRKM theory, transition state theory and our own method. Most results are similar with those of accurate quantum dynamics (QD). At the same time, the RRKM theory, the intramolecular vibration theory, and the vibrational transition state theory for large molecule reaction systems, or the gas-phase reaction kinetics that are difficult to investigate by using accurate quantum dynamics and quasi-classical trajectory method provide the feasibility of estimating. We investigate the anharmonic effect of the canonical and the microcanonical systems, and calculate the total number of states, the density of the states, the partition function and the rate constant. From the various calculation results, we get the following conclusions. First, the anharmonic effect is significant for the weak binding force of microscopic reaction systems. Second, the error of harmonic approximation is larger in high temperature, which is announced for the kinetic mechanism of the combustion reactions. Third, when the molecular reaction is 2000 K, the anharmonic rate constant is smaller than the harmonic rate constant ranging from 2 times to thousands times. The anharmonic effect increases with the increasing temperatures. Fourth, the anharmonic effect is not only related to the intramolecular bond length and binding energy, but also with the symmetry of the molecular structure. We will focus on the developing of an anharmonic model of high-temperature combustion reactions in the following days, high-temperature non-resonant correction calculation methods and apply the method and parameters to building and optimizing the kinetic mechanism of the high-temperature combustion of hydrocarbons.

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**CONTACT (COUNTRY ONLY):** China

**INSTITUTIONS (ALL):** 1. Department of Physics, Dalian Maritime University, Dalian, Liaoning, China.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2227648

**CONTACT (NAME ONLY):** [Thomas Kuntzleman](#)

**TITLE:** [A simple mechanism for fog formation in the dry-ice-in-water experiment](#)

**ABSTRACT BODY:**

**Abstract:** When solid carbon dioxide (dry ice) is placed in water, a cloudy white fog results. It is often assumed that this fog results from atmospheric water vapor condensing on cold carbon dioxide gas that escapes the bulk water. However, simple experiments indicate that this fog originates from the bulk water into which the dry ice is placed. By observing the characteristics of the fogs formed when dry ice is placed in various liquids, insight is gained into the molecular events that lead to fog formation when dry ice is placed in water. Fog formation seems to be related to physical properties of the bulk liquid, such as vapor pressure and surface tension. Additional clues about fog formation in this experiment are gained by viewing high-speed, slow motion video of the fog-filled

bubbles that form at the dry ice / water interface.

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Spring Arbor, MI, United States.  
2. Jackson College, Jackson, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2227328

**CONTACT (NAME ONLY):** [Wendell Dilling](#)

**TITLE:** [How to report the results of an instant run-off election](#)

**ABSTRACT BODY:**

**Abstract:** A clarification of the results of the 2013 ACS President-Elect election was reported in C&EN, March 10, 2014, p 2. The results of that election are shown in the table. The original report in C&EN, November 25, 2013, p 5, reported only total votes for the three candidates, first-choice votes plus second-choice votes for two of the candidates and only first-choice votes for the third candidate. Even though the correct order of finish was reported initially, the total vote counts gave a distorted view of the results. The original report implied that Balazs was supported by 3126 (9638 – 6512) more voters than Kolb was, whereas the difference was only 192 (6704 – 6512) votes. The 42%, 35%, and 23% reported are not pertinent because two of the total vote counts included both first-choice and second-choice votes and the third included only first-choice votes. The last (second in this case) stage of an instant run-off election is between only two candidates (Schmidt and Balazs) and always results in one candidate receiving a majority (>50%) of the votes unless there is a tie. Schmidt received 55% [ $11623 \times 100 / (11623 + 9638)$ ] of the vote in the run-off portion of this election. Kolb was not involved in this second stage. Also the total number of voters, 21659 (8443 + 6704 + 6512), could not be determined from the initial set of numbers reported, which implied 27773 (11623 + 9638 + 6512) voters if one does not recognize that some voters were counted twice.

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, Central Michigan University, Mt. Pleasant, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2227284

**CONTACT (NAME ONLY):** [Wendell Dilling](#)

**TITLE:** [Election of acs directors-at-large by a minority of voters in five of the last six years: A possible solution to the problem, multiple instant run-off voting](#)

**ABSTRACT BODY:**

**Abstract:** In five of the last six years ACS elections for Directors-at-Large (*Chem. Eng. News*, Nov. 23, 2009, p 7; Nov. 28, 2011, p 9; Nov. 26, 2012, p 7; Nov. 25, 2013, p 5; Nov. 24, 2014, p 3) one of the elected candidates received votes from <50% of the voters (Councilors). In each election two Directors-at-Large were elected from a slate of four or five candidates. A method is proposed to carry out elections in which two or more candidates are elected with each being elected by a majority of the voters. The method (multiple instant run-off) involves voters prioritizing their votes. The first Director-at-Large is elected by a majority in exactly the same way a single

candidate would be elected from three or more candidates by the instant run-off procedure. In the instant run-off procedure the candidate with the fewest first-choice votes is eliminated, and the second choice votes on those ballots where the eliminated candidate was the first choice are added to the first choice votes for the other candidates. This procedure is repeated until one candidate has a majority of the votes. Then, in the multiple instant run-off procedure, all the votes for the first candidate elected are removed from the voting priority list of each voter. The second successful candidate is then determined in exactly the same manner as the first using the new prioritized list of each voter. Thus both candidates are elected by a majority in a single election. If more candidates are to be elected, the preceding procedures are repeated.

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, Central Michigan University, Mt. Pleasant, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2209123

**CONTACT (NAME ONLY):** [Ki-Seog Chang](#)

**TITLE:** [Structural study of Mongolian tourmaline in the electric power saving system with infrared spectroscopy](#)

**ABSTRACT BODY:**

**Abstract:** This Fourier Transformation Infrared (FTIR) experiment investigates the relevance of H<sub>2</sub>O and other components' structural environments. Four element materials, tourmaline, ferrite, NaCl, and H<sub>2</sub>O, comprised the electronic power saving system. FTIR spectroscopy in the range of 3,000 to 4,000 cm<sup>-1</sup> was used to examine the hydroxyl ions of H<sub>2</sub>O and Mongolian tourmaline. The tourmaline crystal was polar and therefore pyroelectric, electrical charges developing at the ends of the polar axis and temperature changing from the IR activation with H<sub>2</sub>O in the system. As a result, the tourmaline was shown to be related to the activation of H<sub>2</sub>O as a pyroelectric substance.

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry and Sustainability - Oral

**CONTACT (COUNTRY ONLY):** Korea (the Republic of)

**INSTITUTIONS (ALL):** 1. Bio. & Chemical Engineering, Hongik University, Sejong, Jochiwon-eup, Korea (the Republic of).

**DECISION STATUS:**

**SESSION HOST:** Organizer (Sherine Obare)

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**CONTROL ID:** 2251983

**CONTACT (NAME ONLY):** [Yoseph Daniel](#)

**TITLE:** [Thermal and Flammability Properties of bis-Phosphorus Derivatives of Isosorbide](#)

**ABSTRACT BODY:**

**Abstract:** For applications in printed circuit boards, most traditional flame retardant additives contain bromine and are derived from petroleum. Bromine compounds are coming under increasingly severe regulatory pressure and alternatives are being sought. To generate non-toxic replacements, additives derived from renewable biosources are being developed. In this case, *bis*-phosphorus derivatives of isosorbide have been prepared, fully characterized, and examined as flame-retarding additives in DGEBA epoxy resin. These additives display good polymer compatibility, good thermal stability and enhancement of char formation. The flammability of blends of the

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additives with epoxy resin have been studied using limiting oxygen index (LOI), pyrolysis combustion flow calorimetry (PCFC) and vertical burn (UL94) test methods. Blends of additives (up to 2% phosphorus) with epoxy displayed strongly reduced flammability compared to that for epoxy containing no additives.

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry and Sustainability - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, United States.

2. Center for Applications in Polymer Science, Department of Chemistry, Central Michigan University, Mount Pleasant, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Sherine Obare)

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**CONTROL ID:** 2251346

**CONTACT (NAME ONLY):** [Desmond Murray](#)

**TITLE:** [Calcium Oxide as a Base in Organic Synthesis](#)

**ABSTRACT BODY:**

**Abstract:** Calcium oxide is a cheap, abundant, stable, safe, nontoxic, and environmentally friendly heterogenous base that has been used in organic chemistry. We are currently exploring its applications across a spectrum of base-promoted organic reactions to determine the suitability, effectiveness and versatility of calcium oxide. We will present the results of our work to date.

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry and Sustainability - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Chemistry & Biochemistry, Andrews University, Berrien Sprgs, MI, United States.

2. BEST Early, Berrien Springs, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Sherine Obare)

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**CONTROL ID:** 2251042

**CONTACT (NAME ONLY):** [Richard Taylor](#)

**TITLE:** [Drug Discovery at the University of Notre Dame: The Warren Family Research Center and the Indiana Drug Discovery Alliance](#)

**ABSTRACT BODY:**

**Abstract:** Built upon an historical research strength within the Department of Chemistry & Biochemistry, the University of Notre Dame recently established the Warren Family Research Center for Drug Discovery and Development. The Warren Center is focused towards the discovery and development of new therapeutic leads for the treatment of unmet clinical needs in cancer, infectious disease, stroke, and rare diseases. This collaborative program brings together chemical and biological expertise and technologies to through partnerships with researchers within the biomedically-focused centers at the University of Notre Dame including the Harper Cancer Institute, the Eck Institute for Global Health, the Center for Rare and Neglected Disease and external partners such as the Indiana CTSL. Over the past few years, many of the top research universities have created academic drug discovery programs in an attempt to replicate corporate capability in an academic setting. An alternative approach, like the one being implemented in Indiana, has university-based programs working collaboratively with the pharmaceutical industry to take full advantage of their complementary cultures, expertise, and resources to promote

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early stage discovery and to shepherd potential chemotherapeutic leads through the long and difficult path to the clinic. An overview of the Warren Center at Notre Dame and it's role in the Indiana Drug Discovery Alliance will be presented.

**ABSTRACT SYMPOSIUM NAME:** Academic Drug Discovery: Challenges, Successes, Private Partnerships - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Warren Center for Drug Discovery and the Department of Chemistry Biochemistry, University of Notre Dame, Notre Dame, IN, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Mike Barbachyn)|Organizer (Jed Fisher)

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**CONTROL ID:** 2250904

**CONTACT (NAME ONLY):** [Vera Mainz](#)

**TITLE:** [The Race to Discover Element 61](#)

**ABSTRACT BODY:**

**Abstract:** B Smith Hopkins joined the University of Illinois faculty in 1912. At Illinois, Hopkins conducted research on beryllium, yttrium, columbium (now called niobium), tantalum, and the rare earths. He specialized more and more in the chemistry of the rare earths, which was the field in which he made his greatest contributions to chemistry.

At that time, separating rare earths from each other was a long and tedious process, depending on repeated recrystallizations. In some cases, thousands of recrystallizations were necessary. In 1926, Hopkins with Leonard Yntema and J. Allen Harris announced the discovery of the long sought element 61, which they named "illinium." Hopkins and his co-workers were in a race for this discovery with two other groups: 1) Charles James of the New Hampshire College of Agriculture and Mechanical Arts in Durham, N.H. (in 1923 the University of New Hampshire), who was "scooped" by Hopkins, and 2) Luigi Rolla and Lorenzo Fernandes of the University of Florence, who in 1922, undertook an immense investigation in a search directed at the isolation of element 61, which they dubbed florentium. Rolla contested the precedence of Hopkins' discovery but neither group could duplicate the isolation of element 61. Eventually it was determined that element 61 (now known as promethium) was highly radioactive and did not exist in nature. Hopkins had considered the discovery of illinium the climax of his career, and was bitterly disappointed that his work was not accepted.

**ABSTRACT SYMPOSIUM NAME:** History of Chemistry - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. School of Chemical Sciences, University of Illinois at Urbana-Champaign, Urbana, IL, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Seth Rasmussen)

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**CONTROL ID:** 2250784

**CONTACT (NAME ONLY):** [Desmond Murray](#)

**TITLE:** [Research From High School to Grad School](#)

**ABSTRACT BODY:**

**Abstract:** Not many teachers have the opportunity to concurrently engage high school through graduate school

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students in research. This presentation will describe approaches used and experiences had along the continuum of guided inquiry to independent research.

**ABSTRACT SYMPOSIUM NAME:** High School, Community College, and Undergraduate Education - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Chemistry & Biochemistry, Andrews University, Berrien Sprgs, MI, United States.  
2. BEST Early, Berrien Springs, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Thomas Higgins)

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**CONTROL ID:** 2250481

**CONTACT (NAME ONLY):** [Zachary Swingen](#)

**TITLE:** [Modification and Green Synthesis of Sustainable Tri-block Copolymers](#)

**ABSTRACT BODY:**

**Abstract:** The importance of green polymer synthesis and sustainable polymers is the focus in a new experiment developed as a guided-inquiry polymer lab for undergraduate organic chemistry courses at all types of institutions. The lab highlights the fact that the various incorporation of monomers derived from renewable feedstocks, such as *L*-lactide,  $\delta$ -dodecalactone, and dodecalactone, are related to the physical and mechanical properties the polymer displays. This experiment not only introduces students to the fundamentals of polymer chemistry, but also instills quantitative data analysis techniques through analysis of  $^1\text{H}$ -NMR spectra of the synthesized polymer to calculate the composition and molecular weight of the product.

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Augsburg College, Roseville, MN, United States.  
2. Chemistry, Augsburg College, Minneapolis, MN, United States.  
3. Chemistry, University of Minnesota, Plymouth, MN, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2250408

**CONTACT (NAME ONLY):** [Alan Medina-Gonzalez](#)

**TITLE:**

[Continuous Flow Chemistry for the Synthesis of Amides from Nitriles and Amines](#)

**ABSTRACT BODY:**

**Abstract:**

Amide bonds are a significant functional group of biological relevance in peptides and proteins, which are significant to pharmaceutical drugs. Amides are formed conventionally in condensation reactions using an amine and carboxylic acid in the presence of strong acid, forcing conditions, and from the acid chloride. However, usages of these chemicals can be highly expensive, waste generating, and less efficient. We have developed an alternative method to produce amides using a continuous flow reactor that is composed of a HPLC column packed with a titanium dioxide catalyst. Numerous variables such as flow rate, temperature, and pressure can be investigated rapidly with

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this method. By using phenylacetylnitrile, a benzylic nitrile, and various amines numerous amides have been synthesized.

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Augsburg College, Roseville, MN, United States.  
2. Chemistry, Augsburg College, Minneapolis, MN, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2250048

**CONTACT (NAME ONLY):** [Erika Olbricht](#)

**TITLE:** [Only Culinary?: Early modern medicinal uses of spice](#)

**ABSTRACT BODY:**

**Abstract:** Current alternative medicinal practice includes many plant-based remedies, but many of these plants and the knowledge about their medicinal properties are ancient. This paper explores what early English herbalists knew about spices and the plants that produce them, and in doing so, will also refer to classical writers, especially Galen and Dioscorides, who were important to early English herbalists. While today, we are likely to make distinctions between culinary and medicinal uses of various plants, there are several instances in early periods that show they did not make such distinctions. For example, at medieval feasts, often courses were served in order of the food's Galenic properties: hot and moist foods were generally followed by cold and dry foods. There is also evidence that such meals included plates of spices alongside the final course that were eaten to aid digestion. While this paper draws on scholarly work about the role of spices in culture and trade, it focuses primarily on the use of black pepper as a culinary spice and object of trade, but primarily as an herbal remedy—as a hot, dry choleric spice, it played a particular role in the physiological balance of the humors and was an expensive, prized spice often kept under lock and key.

**ABSTRACT SYMPOSIUM NAME:** Health Benefits of Natural Products in Spices: The Past, Present and Future - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. English, Case Western Reserve University, Cleveland, OH, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Raul Juarez)

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**CONTROL ID:** 2249929

**CONTACT (NAME ONLY):** [Hongshan He](#)

**TITLE:** [Acyclic acid functionalized porphyrins for dye-sensitized solar cells](#)

**ABSTRACT BODY:**

**Abstract:** Dye-sensitized solar cell (DSC) is an electrochemical device that has a great potential to convert solar energy into electricity cost-effectively. Dyes are of importance to DSCs. Among numerous dyes investigated, porphyrins have emerged as one type of most efficient dyes for DSCs. Presently, a donor- $\pi$ -acceptor structure has been identified as a premium model for porphyrin-sensitized solar cells. In this model, a donor is usually a diphenylamine derivative, and an acceptor is an ethynylbenzoic acid in two opposite meso positions of a porphyrin ring. Though the energy efficiency up to 13% has been reported, it is still challenging to broaden the absorption capability to a longer wavelength. In this study, we designed and synthesized several porphyrin dyes with an

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acrylic acid as an acceptor. This design shortened the distance between porphyrin dye and titanium dioxide nanoparticle surface; therefore could facilitate the electron injection to increase the energy conversion efficiency. The detailed synthesis, characterization, photophysical and photovoltaic measurements will be presented.

**ABSTRACT SYMPOSIUM NAME:** General Call for Papers Inorganic Chemistry - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Chemistry, Eastern Illinois University, Charleston, IL, United States.  
2. School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou, Guangdong, China.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Brian Eklov)

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**CONTROL ID:** 2249836

**CONTACT (NAME ONLY):** [Kerry Rouhier](#)

**TITLE:** [Results from an external review of the Kenyon College Summer Scholars Program: an ongoing discussion between faculty and administration](#)

**ABSTRACT BODY:**

**Abstract:** Undergraduate research in the sciences has been an integral part of applied learning at Kenyon College for more than 30 years. Students participate as "... partners in inquiry..." (Kenyon's mission statement) during the academic year and throughout the summer. This academic year, the Department of Chemistry has more than thirty students working in our labs on various projects as volunteers or for course credit. During the summers, students apply to participate in our Kenyon Summer Science Scholars program (KSSS). What started as a small research program funded through external grants (NSF, NIH, and HHMI), the KSSS program is now entirely supported by the college. More than thirty students and their faculty mentors are provided stipends to conduct research for 8-10 weeks each summer. Student-faculty teams hail from all departments in the Natural Science Division (Chemistry, Physics, Biology, Mathematics and Statistics, and Psychology) and the Department of Anthropology. In 2014, members of the KSSS program conducted a thorough self-study and underwent an external review. We sought feedback in these broad areas- 1) meeting the needs of the students, 2) meeting the needs of the faculty, and 3) best practices for a sustainable and high-quality program. I will be sharing the results of our Review, including feedback from our subsequent discussions with the administration.

**ABSTRACT SYMPOSIUM NAME:** Research at Undergraduate Institutions - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Chemistry Department, Kenyon College, Gambier, OH, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Bradley Wile)

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**CONTROL ID:** 2248760

**CONTACT (NAME ONLY):** [Steven Tanis](#)

**TITLE:** [A New Class of mTOT-Modulating Thiazolidinedione Insulin Sensitizers](#)

**ABSTRACT BODY:**

**Abstract:** Early thiazolidine (TZD)-containing antidiabetic agents such as ciglitazone, pioglitazone (Actos®), rosiglitazone (Avandia®), and troglitazone (Rezulin®) were all discovered empirically, as a result of whole animal testing. Consistent with the Medicinal Chemistry drumbeat for a defined mechanism, the mid-1990's saw a strong case being made that these compounds exerted their activity by a direct activation of the nuclear transcription factor

peroxisome proliferator-activated receptor  $\gamma$  (PPAR $\gamma$ ). This testing paradigm led to numerous, potent PPAR $\gamma$  activators (and dual PPAR $\alpha/\gamma$  activators) entering development without success. Over the past 10 years or so evidence for a mitochondrial target for TZD's has emerged, called mTOT (*mitochondrial target of thiazolidinediones*), with PPAR activation associated with the undesired effects (weight gain, increase in intravascular volume, peripheral oedema, and congestive heart failure), this new mitochondrial target provided a potential new approach diseases associated with insulin resistance. A medicinal chemistry program targeting antidiabetic activity with a greatly reduced PPAR $\gamma$  liability while maintaining the insulin sensitizing pharmacology led to the selection of **MSDC-0160** and **MSDC-0602** for development. These compounds have active metabolites with further reduced capability to activate PPAR $\gamma$ . To date, these compounds have been through Phase 2b clinical development and they exhibit insulin sensitizing pharmacology similar to pioglitazone (Actos®) without the adverse effects associated with PPAR $\gamma$  agonists thus providing a new approach for treating metabolic diseases.

**ABSTRACT SYMPOSIUM NAME:** Upjohn, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. SPTanis PharmaChem Consulting LLC, Carlsbad, CA, United States.

2. Metabolic Solutions Development Company, Kalamazoo, MI, United States.

3. Kalexsyn, Portage, MI, United States.

4. Department of Medicinal Chemistry, College of Pharmacy, University of Michigan, Ann Arbor, MI, United States.

5. Jim Zeller Consulting LLC, Scottsdale, AZ, United States.

6. Kalexsyn, Portage, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Jed Fisher)|Organizer (Mike Barbachyn)

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**CONTROL ID:** 2248542

**CONTACT (NAME ONLY):** [Brandon Bowser](#)

**TITLE:** [Investigating the foundational layer formation of metal-organic coordinated thin films](#)

**ABSTRACT BODY:**

**Abstract:** This research explores layer-by-layer (LBL) assembly for two types of metal-organic coordinated thin films, multilayers (ML) and frameworks (MOF). Controlled step-wise assembly defines the resulting film structure, presenting an opportunity to design these materials for specific applications, such as sensing and gas storage. Towards this realization, both films are fabricated by alternating, sequential solution phase deposition. Both systems were synthesized beginning with a 16-mercaptohexadecanoic acid (MHDA) self-assembled monolayer on gold. ML were composed of  $\alpha,\omega$ -mercaptoalkanoic acids and Cu (II) ions forming a conformal film. MOF were composed of 1,3,5-benzenetricarboxylic acid and Cu (II) ions (HKUST-1) yielding a porous crystalline framework. Both films were characterized using ellipsometry to measure film thickness and scanning probe microscopy (SPM) to map topographical morphology of film growth LBL. Using image analysis software, quantitative data regarding the growth of these thin films based on the images was procured (e.g. Particle Analysis and Percent Area Coverage). Ellipsometry suggests both ML and MOF form continuous, conformal layers that are each about 2 nm thick, respectively. However, SPM images elucidate two distinct systems, one that forms a semi-continuous film with distinct "islanding" (ML) and one that forms a rough surface of nucleating crystallites (MOF). The effects of deposition conditions, such as temperature and solution concentration, have been investigated in order to tailor film morphology for specific applications. Preliminary findings will be presented for utilizing infrared spectroscopy to study gas absorption within the MOF. Future work includes observing continued MOF growth to monitor at what point it becomes continuous and to investigate how the film forms beyond the threshold of complete surface coverage. Further studies will investigate other metal-organic coordinated thin film systems to understand the chemical and physical processes by which different film morphologies arise.

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**CONTACT (COUNTRY ONLY):** United States

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**INSTITUTIONS (ALL):** 1. Hope College, Midland, MI, United States.  
2. Chemistry, Hope College, Holland, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2248057

**CONTACT (NAME ONLY):** [Roger Dekock](#)

**TITLE:** [Theoretical interpretation of atomic and ionic size](#)

**ABSTRACT BODY:**

**Abstract:** Central to an understanding of electronic behavior upon ionization of atoms is the concept of atomic and ionic size. This concept is qualitative, resulting in many different ways of calculating the “radius” of an atom. Our lab has utilized the quantum chemistry software GAMESS to model the electron densities of atoms and their ions in order to calculate theoretical radii. We are interested in two groups of these radii, those that align more closely with covalent radii, and those that align with van der Waals radii, both of which are derived from experiment. Our results show that a single theoretical calculation method does not correlate with both experimentally-derived atomic and ionic radii.

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Calvin College, Grand Rapids, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2247067

**CONTACT (NAME ONLY):** [Jonathan Derouin](#)

**TITLE:** [Adsorption of atomic oxygen on Ag\(111\)](#)

**ABSTRACT BODY:**

**Abstract:** Understanding the interaction of oxygen with transition metal surfaces is important in many areas including corrosion and catalysis. The oxygen/silver system in particular has been studied extensively both experimentally and theoretically. Interest is driven largely by the role of silver in two widely used industrial reactions: the epoxidation of ethylene to produce ethylene oxide and the partial oxidation of methanol to produce formaldehyde. The oxygen/silver system can also serve as a model for the dissociative chemisorption of diatomic molecules on close packed metal surfaces. Despite extensive research, the oxygen/silver system is still not well understood. To better understand this system, we use UHV-STM, AES and TPD to study the adsorption of atomic O on an Ag(111) crystal. Atomic O is generated by thermally cracking O<sub>2</sub>. By varying the power of the thermal cracker we are able to change the flux and energy of atomic O reaching the Ag surface. Using lower power, in addition to large p(4x4), p(4x5√3), c(3x5√3), and c(4x8) domains, a previously unseen adsorbate structure was identified. When higher power was used to thermally crack O<sub>2</sub>, another oxide structure with a significantly higher temperature desorption peak was formed. All of the adsorbate structures were characterized using AES, TPD and STM.

**ABSTRACT SYMPOSIUM NAME:** Catalysis and Surface Science to Advance Energy Efficiency - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Loyola University Chicago, Chicago, IL, United States.

2. Chemistry, Loyola University Chicago, Palatine, IL, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Daniel Killelea)

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**CONTROL ID:** 2246175

**CONTACT (NAME ONLY):** [Jacob Ciszek](#)

**TITLE:** [Molecular crystals: A different take on surface science](#)

**ABSTRACT BODY:**

**Abstract:** Science naturally gravitates towards well-defined systems of societal relevance. As such, the field of surface science arose from classical elemental surfaces and industrially relevant systems (e.g. silicon and catalytic surfaces). But as technologies change, new materials beckon to inquisitive scientists. As such, we have been recently studying organic semiconductors, with a surface chemistry as robust as their predecessors, and applications across all modes of electronic devices. We find that both single crystal and polycrystalline organic substrates are amenable to surface functionalization, and that many of the classical surface science tools (XPS, PM-IRRAS, etc.) can elucidate the structural features (density, chemical bonding, etc.) of these reacted surfaces. Interestingly, the unique composition of the surface (anisotropic building blocks held together by intermolecular forces) results in many features not displayed by traditional systems, including extreme differences in reactivity of the various facets.

**ABSTRACT SYMPOSIUM NAME:** Catalysis and Surface Science to Advance Energy Efficiency - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, Loyola University, Chicago, IL, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Daniel Killelea)

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**CONTROL ID:** 2244148

**CONTACT (NAME ONLY):** [Colin Agatisa-Boyle](#)

**TITLE:** [The effect of polyphenols on abeta aggregation](#)

**ABSTRACT BODY:**

**Abstract:** Alzheimer's Disease, which is caused partially by the aggregation of the abeta peptide, is a major and growing public health concern. The abeta peptide initially exists in a monomeric random coil configuration, but transitions into a beta sheet conformation and oligomerizes as it aggregates. This presentation will examine if natural products could play a role in treating Alzheimer's Disease. Polyphenols from spices such as resveratrol, curcumin and capsaicin can potentially inhibit the aggregation of the abeta peptide. Circular dichroism was used to track the secondary structure conformation change of the peptide. NMR techniques were used to examine the interactions of the natural products with specific amino acids of abeta. Finally, atomic force microscopy was used to observe oligomer and fibril formation of abeta controls versus abeta treated with the various natural products.

**ABSTRACT SYMPOSIUM NAME:** Health Benefits of Natural Products in Spices: The Past, Present and Future - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Chemistry, Case Western Reserve University, Shaker Heights, OH, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Raul Juarez)

**CONTROL ID:** 2242347

**CONTACT (NAME ONLY):** [SydneyChanel Price](#)

**TITLE:** [Hydrogenation of tetraphenylcyclopentadione](#)

**ABSTRACT BODY:**

**Abstract:** This experiment is a hydrogenation reaction using Tetraphenylcyclopentadione. The Tetraphenylcyclopentadione will be reacting with  $H_{2(g)}$  and 5% Pd/C in  $CH_2CL_2$ . The starting material is purple solid and the reaction creates a different white solid. Analysis of the reactions will be done by testing in IR and TLC analysis. The hydrogen adds anti but because of the metal center it should add syn. The experiment also should yield a trans-product but it makes a cis-product. I will change the source of hydrogen using gas and ammonium formate to find out if that makes a difference.

Ref. Mohrig, J. R.; Hammond, C. N.; Schatz, P.F.; Davidson, T. A. J. *Chem. Ed.* **2009**, 86, 243-239

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Detroit, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2242205

**CONTACT (NAME ONLY):** [Haley Coggins](#)

**TITLE:** [Synthesis of pyrido lentzium](#)

**ABSTRACT BODY:**

**Abstract:** The focus of this experiment is to change a dianhydride into a diimide product. This will be done using 4-aminomethyl piperidine and imidazole as a catalyst. The energy supply for the procedure will come from heated air. The goal of this experiment is to verify the synthesis of the target molecule, and to attempt to increase the yield and purity of the compound through recrystallization.

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Spring Arbor, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2242075

**CONTACT (NAME ONLY):** [Zhong-Yin Zhang](#)

**TITLE:** [Drugging the undruggable: Therapeutic potential of targeting the protein tyrosine phosphatases](#)

**ABSTRACT BODY:**

**Abstract:** Aberrant tyrosine phosphorylation has been linked to the etiology of many human diseases including

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cancer, diabetes/obesity, neurodegenerative and autoimmune disorders. Notable success has been achieved in targeting signaling pathways regulated by protein tyrosine phosphorylation, with more than a dozen of small molecule kinase inhibitors already in the clinic. However, despite the fact that protein tyrosine phosphatases (PTPs) have been garnering attention as potential therapeutic targets, they remain largely an untapped resource. In fact, PTP-based drug discovery programs have historically been shrouded with difficulty in inhibitor selectivity and bioavailability, both of which are related to the intrinsic PTP active site properties.

We apply a novel approach for the design of potent and specific PTP inhibitors by tethering appropriately functionalized moieties to a nonhydrolyzable pTyr mimetic in order to engage both the active site and nearby unique peripheral binding pockets. By targeting less conserved interactions outside of the pTyr-binding cleft, increased affinity and selectivity can be obtained. Several novel nonhydrolyzable pTyr mimetics have been developed over the last few years offering potential solutions to overcome the bioavailability issue that has long plagued the PTP drug discovery field. Our recent work demonstrate that phosphonodifluoromethyl phenylalanine (F<sub>2</sub>Pmp), a well-established nonhydrolyzable pTyr surrogate, and bicyclic salicylic acid pharmacophores are sufficiently polar to bind the PTP active site, yet remain capable of efficiently crossing cell membranes, offering PTP inhibitors with both high affinity and selectivity and excellent *in vivo* efficacy in animal models of oncology, diabetes/obesity, autoimmunity, and tuberculosis. Current work is focused on advancing our lead generation paradigms and create a 'PTP-based drug discovery platform' that will ultimately impact broadly the portfolio of tomorrow.

**ABSTRACT SYMPOSIUM NAME:** Academic Drug Discovery: Challenges, Successes, Private Partnerships - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Biochemistry and Molecular Biology, Indiana University School of Medicine, Carmel, IN, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Mike Barbachyn)|Organizer (Jed Fisher)

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**CONTROL ID:** 2239410

**CONTACT (NAME ONLY):** [Elizabeth Brueggeman](#)

**TITLE:** [Synthesis of glycine phthalimide using a heat gun](#)

**ABSTRACT BODY:**

**Abstract:** Reactions between phthalic anhydride and various amides to create imide acids were studied. A heat gun was used to supply energy to drive the reaction. Phthalic anhydride and glycine reacted to produce glycine phthalimide. Because it has been observed that energy from microwave ovens increases the rates of these reactions (1), a study of the effect of the energy supplied by the heat gun on the control of the reaction will be conducted. In addition to glycine, other amides may be used as reactants in this study. References: 1. Bari, S., Bose, A., Chaudhary, A., Manhas, M., Raju, V., & Robb, E. Reactions Accelerated by Microwave Radiation in the Undergraduate Organic Laboratory. J. of Chem. Ed., 1992, 69, 938-939.

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Jackson, MI, United States.  
2. Spring Arbor University, Spring Arbor, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**CONTROL ID:** 2236963

**CONTACT (NAME ONLY):** [Rachael Farber](#)

**TITLE:** [Water adsorption on Pt\(111\) and stepped Pt surfaces](#)

**ABSTRACT BODY:**

**Abstract:** The interaction of water with metal surfaces has attracted much attention in the field of surface science. Water is ubiquitous on earth and is therefore of high significance to a wide range of fields, from studies of material aging and corrosion to atmospheric science. Studies of the adsorption, wetting, and desorption of water on metal surfaces continues to reveal new, and sometimes surprising, information about this deceptively simple system. Most relevant to this work are more recent advances in understanding the structures formed by submonolayer coverages of water on metal surfaces. Progress in this avenue has been facilitated by a combination of atomically resolved imaging experiments with density functional theory (DFT) calculations to elucidate how the balance of the water-water and water-surface interactions yield the bonding patterns and behavior of water on regular metal surfaces [1]. As the application of these methods continues to develop, the understanding of 2-D water cluster formation and bonding behavior has given greater insight into the unique chemistry displayed by water on metal surfaces

Thus far, most studies have focused on the interaction of water with flat, regular metal surfaces; the still emerging studies of water on terrace step edges has further added to this already rich field [2]. In this project, we will study the arrangements of small clusters of water molecules on highly stepped Pt surfaces and compare the submonolayer coverage clusters on the stepped surfaces to those found on planar surfaces. We begin our study by first imaging water clusters on a Pt(111) crystal surface using an ultra-high vacuum scanning tunneling microscope (UHV-STM). We will then move on to studying the stepped surfaces. We will compare our observations to the predictions from DFT calculations of the same system [3]. The information gathered in this project will not only give further insight into water's unique behavior on metal surfaces, but also provide information on water's behavior on more reactive surface sites. An understanding of how steps and defects perturb the delicate balance of water-water and water-substrate interactions will result from this study.

**References:**

- [1] A. Hodgson; S. Haq; *Surf. Sci. Rep.* **64** 381 (2009).
- [2] M. van der Niet; A. den Dunnen; L.B.F. Juurlink; M.T.M. Koper; *PCCP* **13** 1629 (2011)
- [3] M.J. Kolb; F. Calle-Vallejo; L.B.F. Juurlink, M.T.M. Koper; *JCP* **140** 134708 (2014)

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Loyola University Chicago, Chicago, IL, United States.  
2. LIC / CASC, University Leiden, Leiden, Zuid Holland, Netherlands.  
3. Leiden Institute of Chemistry, Leiden, Netherlands.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2235959

**CONTACT (NAME ONLY):** [George Bodner](#)

**TITLE:** [An international perspective on green chemistry and sustainability education](#)

**ABSTRACT BODY:**

**Abstract:** The literature on Green Chemistry and Sustainability (or Sustainable Development) suggests that these terms are often used as if they were synonymous. The results of a Symposium on Science Education Research and Education for Sustainable Development held at the University of Bremen, last summer, clearly showed that they are not. This paper will use the results of this symposium to look at efforts to bring Green Chemistry and/or Sustainability Education into the chemistry curriculum under the context of "relevance" in diverse cultures around

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the world. If time permits, the author will also reflect on a recent study done by the ACS Green Chemistry Institute of the state of Green Chemistry education in the U.S.

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry and Sustainability - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Dept of Chemistry, Purdue University, W Lafayette, IN, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Sherine Obare)

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**CONTROL ID:** 2231671

**CONTACT (NAME ONLY):** [Jennifer Batten](#)

**TITLE:** [Integrating gas chromatography-mass spectrometry into organic chemistry to improve student interest in and skill with this technique and beyond](#)

**ABSTRACT BODY:**

**Abstract:** The recent acquisition of a gas chromatograph-mass spectrometer (GC-MS) through the National Science Foundation Grant DUE 1140509 has allowed the faculty at Grand Rapids Community College to incorporate this instrument across the two-year curriculum. This technique was used in the organic chemistry lab sequence to highlight the mass spectrometry data of functional groups and to introduce basic quantitative methods. With the goal of improving interest in and comprehension of a variety of chemistry related topics including cation stability and resonance, seven experiments were adapted or developed to include GC-MS. The methods and outcomes of this work will be presented including curriculum development, student feedback, and assessment of student achievement.

**ABSTRACT SYMPOSIUM NAME:** High School, Community College, and Undergraduate Education - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Physical Sciences, Grand Rapids Community College, Jenison, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Thomas Higgins)

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**CONTROL ID:** 2231232

**CONTACT (NAME ONLY):** [Yirong Mo](#)

**TITLE:** [The directionality of non-covalent bonds](#)

**ABSTRACT BODY:**

**Abstract:** The recently proposed s-hole concept by Clark, Politzer and their coworkers not only reinforces the contribution of electrostatic attraction to non-covalent bonds, but implies the angular dependency of the electrostatic force. To probe the magnitude of covalency, i.e., the electron transfer interaction, and its contribution to the directionality in non-covalent bonding, we investigated a small group of exemplary molecules which include hydrogen bonding, halogen bonding, chalcogen bonding and pnictogen bonding systems. The computational study is based on the block-localized wavefunction (BLW) method which decomposes the binding energy into the steric energy, which is a combination of electrostatic, Pauli repulsion, polarization and electron correlation effects, and the electron transfer (hyperconjugation) energy. The uniqueness of the BLW method is that it can provide optimal geometries with only steric effect included but electron transfer interaction excluded. On one hand, computations show that when only steric effect rules with the electron transfer interaction quenched, the bonding distances are about 0.5–0.8 Å shorter than the sum of van der Waals atomic radii due to the electrostatic attraction, and the overall steric effect exhibits the angular dependency notably in halogen bonding, chalcogen bonding and pnictogen

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bonding systems. On the other hand, the electron transfer interaction significantly shortens non-covalent bonding distances. This bond shortening enhances the Pauli repulsion which subsequently offsets the electrostatic attraction, and in the end the contribution of the steric effect to bonding is diminished. For instance, in the halogen bonding system  $H_3N \cdots ClF$ , the steric effect is even destabilizing and the binding is completely contributed by the electron transfer interaction. In several other systems particularly hydrogen bonding systems, the steric effect nevertheless still plays the major role while the electron transfer interaction is minor. However, in all cases, the electron transfer exhibits strong directionality, suggesting that the linearity or near linearity of non-covalent bonds is largely governed by the electron transfer interaction whose magnitude determines the covalency in non-covalent bonds.

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Western Michigan University - Mailstop 5413, Kalamazoo, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2231227

**CONTACT (NAME ONLY):** [Yirong Mo](#)

**TITLE:** [Combined QM/MM study of the isomerization of 1-Deoxy-D-Xylulose 5-Phosphate \(DXP\) catalyzed by DXP reductoisomerase \(DXR\)](#)

**ABSTRACT BODY:**

**Abstract:** The conversion of 1-deoxy-D-xylulose 5-phosphate (DXP) to 2-C-methyl-D-erythritol 4-phosphate (MEP) catalyzed by DXP reductoisomerase (DXR) is the committing step in the biosynthesis of terpenoids. This MEP pathway is essential for most pathogenic bacteria but absent in human, thus is an attractive target for the development of novel antibiotics. To this end, it is critical to elucidate the conversion mechanism and identify the transition state, as many drugs are transition state analogues. Here we performed extensive combined quantum mechanical (density functional theory B3LYP/6-31G\*) and molecular mechanical molecular dynamics simulations to elucidate the catalytic mechanism. Computations confirmed the transient existence of two metastable fragments of DXP by the heterolytic C3-C4 bond cleavage, namely 1-propene-1,2-diol and glycoaldehyde phosphate, in accord with the most recent kinetic isotope effect (KIE) experiments. Significantly, the heterolytic C3-C4 bond cleavage and C2-C4 bond formation are accompanied by proton shuttles, which significantly lower their reaction barriers to only 8.2-6.0 kcal/mol, compared with the normal single carbon-carbon bond energy 83 kcal/mol. This mechanism thus opens a novel way for the design of catalysts in the cleavage or formation of aliphatic carbon-carbon bonds.

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Western Michigan University - Mailstop 5413, Kalamazoo, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2230995

**CONTACT (NAME ONLY):** [Jeffrey Johnson](#)

**TITLE:** [Rhodium-catalyzed C-C single bond activation: Using mechanistic understanding to guide reaction development](#)

**ABSTRACT BODY:**

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**Abstract:** Methodology achieving the activation and functionalization of carbon-carbon single bonds holds the promise to unveil previously unforeseen retrosynthetic disconnects. This presentation will summarize ongoing mechanistic investigations of rhodium-catalyzed carbon-carbon bond activation methodologies and outline successful efforts to utilize the resulting quantitative insight to develop new transformations.

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Hope College Chemistry Dept, Holland, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Jay Wackerly)

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**CONTROL ID:** 2230854

**CONTACT (NAME ONLY):** [Wendell Dilling](#)

**TITLE:** [Enantiodifferentiating \[4+4\] photocyclodimerization of 2-Anthracene-carboxylate catalyzed by 6<sup>A</sup>,6<sup>X</sup>-Diamino-6<sup>A</sup>,6<sup>X</sup>-dideoxy- \$\gamma\$ -cyclodextrins: Misinterpretation of the sign of differential entropy of activation](#)

**ABSTRACT BODY:**

**Abstract:** Inoue and coworkers reported the title reactions in which the four dimers **1-4** are formed (*J. Photochem. Photobiol. A: Chem.* **2005**, *173*, 375-383). The relative yields of dimers **1-4** and the enantiomeric excesses of dimers **2** and **3** (as high as 37%) could be controlled within limits by varying the catalyst, temperature, and solvent composition. Linear plots of the relative rate constants for the formation of the enantiomers of **3** against the reciprocal temperature in various concentrations of aqueous methanol gave data from which the differential enthalpy of activation and the differential entropy of activation could be calculated. These authors report the signs (+ or -) of these differential activation parameters. The absolute values of these signs are completely arbitrary. Only the relative values have significance.

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, Central Michigan University, Mt. Pleasant, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2230847

**CONTACT (NAME ONLY):** [Deepti Dabas](#)

**TITLE:** [Natural Colors for Food and Beverages](#)

**ABSTRACT BODY:**

**Abstract:** Color is the most important component influencing the purchase of food. Colors are added to food for consistency and to meet customer expectations among other reasons. Natural Colors are coming to the forefront replacing synthetics. Natural colors, with the use of appropriate technology and know-how of applications, can perform at par with synthetics. Different pigments can provide with different hues required for color match. Carrot and turmeric provide yellow color to foods with the coloring pigments being beta-carotene and curcuminoids respectively. Annatto can be used as yellow or orange colorant depending on concentration and application, with the active component being bixin. Paprika can provide a red or orange hue to foods, owing to compounds-capsorubin and capsanthin. Anthocyanins are a bigger class of compounds with pigments providing different hues in red-purple family depending on their structure. Betalains and lycopene can also provide red colors isolated

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respectively from beet and tomatoes. Chlorophyll is the green colored pigment but is not allowed for use in the USA. Depending on desired hue, the physical properties of pigments can be changed or suitable stabilizers can be added which impart better performance. Depending on the nature of pigments, two or more pigments can be mixed to provide the desired color. Knowing about application matrix is very important for the pigment to perform successfully in that application. Today natural colors are growing fast as more and more consumers are seeking them over synthetic colorants.

**ABSTRACT SYMPOSIUM NAME:** Color Your Food: Meeting the Challenges of Natural Food Colors - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Colors, Kalsec, Kalamazoo, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Shane McDonald)

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**CONTROL ID:** 2229237

**CONTACT (NAME ONLY):** [Krisanu Bandyopadhyay](#)

**TITLE:** [Silver nanoshells synthesis by \*in situ\* generation of silver seeds on silica nanoparticle cores](#)

**ABSTRACT BODY:**

**Abstract:** Recently, several differing core-shell combinations of nanoshells have been fashioned by the bottom-up approach and are finding prospective applications in cancer treatment as well as solar energy absorbers. The synthesis procedure to generate this silica nanoparticle is well documented in literature. Most metal nanoshells such as gold and palladium have been published. Silver nanoshells are still a work in progress. Silver nanoparticles are known for its anti-bacterial properties, that are beneficial for the health of human being. Currently, silver seeds are formed externally and then adsorbed onto a surfactant functionalized silica core surface which then proceed to its final growth stage. The present research deals with a more efficient method of synthesizing these silver nanoshells by eliminating the need of pre-synthesized silver seed in solution. The reason for a different method is to help shorten the overall synthesis process. This efficient route to generating silver nanoshells will improve their candidacy for various potential applications in the medical field and solar energy harvesting.

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Department of Natural Sciences , University of Michigan-Dearborn, Dearborn, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2229235

**CONTACT (NAME ONLY):** [Krisanu Bandyopadhyay](#)

**TITLE:** [Catalytic assessment and characterization of \*in-situ\* generated gold-palladium bimetallic nanoparticles on functionalized surfaces](#)

**ABSTRACT BODY:**

**Abstract:** The use of nanoparticle-based heterogeneous catalysts has grown immensely in recent years due to their high surface area and unique chemical and physical properties. While many noble metal nanoparticles (such as gold, platinum, palladium, and silver) have proven to be promising catalytic systems, a combination of these materials may prove to be an even better option, combining the advantages of each metal individually. The present work involves the *in-situ* generation of 2D gold-palladium (Au-Pd) bimetallic nanoparticle assemblies on

functionalized silicon and indium-tin oxide (ITO) coated glass substrates. Varying ratios of gold and palladium are used to produce a set of catalysts, ranging from only gold to only palladium. Atomic Force Microscopy (AFM) is used to characterize the physical structure of the nanoparticles while zeta potential measurements are used to track the change in surface charge throughout the generation process. UV-Visible (UV-Vis) spectroscopy is used to observe the optical properties of the bimetallic nanoparticles, giving insight to their morphology. The catalytic properties of the nanoparticle arrays are assessed electrochemically through the oxidation of ethanol and ethylene glycol using cyclic voltammetry. Additionally, the catalytic abilities of these bimetallic nanoparticles assemblies are assessed through the catalytic reduction of 4-nitrophenol to 4-aminophenol in the presence of excess borohydride. This reaction is monitored through UV-Visible response, allowing for the calculation of the apparent rate constants of the reaction. Through the use of these various characterization techniques, we hope to understand the morphology of these nanostructures and tune their catalytic abilities.

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Department of Natural Sciences , University of Michigan - Dearborn , Canton , MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2229131

**CONTACT (NAME ONLY):** [Krisanu Bandyopadhyay](#)

**TITLE:** [Non-enzymatic glucose biosensing using gold nanoparticles](#)

**ABSTRACT BODY:**

**Abstract:** Diabetes is a common long term disorder characterized by high blood glucose concentration. Commonly known ways of detecting glucose levels involve the enzymatic approach of undergoing rapid redox reactions with Glucose Oxidase (GOx) and a small mediator molecule such as ferrocyanide or other ferrocene derivatives. Furthermore, there are other known ways of detecting glucose but all methods require the GOx enzyme. The issues involving stability of this enzyme leads to a short shelf life in the products used to detect blood glucose concentrations. The present research identify a non-enzymatic way of glucose sensing that excludes the need of any mediator and GOx, subsequently reducing costs and eliminating conditions required to keep GOx stable during sensing process. We have used our own method to generate in situ gold nanoparticles assemblies on indium tin oxide (ITO) coated glass surfaces. These newly synthesized gold nanoparticles is used as sensing platform in conjunction with electrochemical impedance spectroscopy and cyclic voltammetry to measure electrochemical response with varying concentration of glucose to probe for a linear range between concentration and electrochemical parameters. Fitting Impedance response to an appropriate equivalent circuit shows an increase in inverse of charge transfer resistance with increasing glucose concentrations which reveal a systemic non-enzymatic method of detecting glucose with two dimensional assemblies of gold nanoparticles. Additionally, cyclic voltammograms show a consistent trend of increasing current with increase in glucose concentration that supports the general applicability of this method of glucose sensing.

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. University of Michigan-Dearborn, Dearborn, MI, United States.

2. Department of Natural Sciences , University of Michigan - Dearborn , Dearborn, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**CONTROL ID:** 2229075

**CONTACT (NAME ONLY):** [E Charles Sykes](#)

**TITLE:** [Single atom alloys as a strategy for selective heterogeneous hydrogenations](#)

**ABSTRACT BODY:**

**Abstract:** Hydrogenation reactions are central to the petrochemical, fine chemical, pharmaceutical, and food industries and are of increasing interest in energy production and storage technologies. Typical heterogeneous catalysts often involve noble metals and alloys based on platinum, palladium, rhodium and ruthenium. While these metals are active at modest temperature and pressure, they are not always completely selective and are expensive. We have demonstrated that single palladium atoms can convert the otherwise catalytically inert surface of an inexpensive metal into an ultrasensitive catalyst. We used high resolution imaging to characterize the active sites and temperature programmed reaction spectroscopy to probe the chemistry. The mechanism involves facile dissociation of molecular hydrogen at individual palladium atoms followed by spillover onto the copper surface, where ultrasensitive catalysis occurs by virtue of weak binding. The reaction selectivity is in fact much higher than that measured on palladium alone, illustrating the unique synergy of the system.

**ABSTRACT SYMPOSIUM NAME:** Catalysis and Surface Science to Advance Energy Efficiency - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Tufts University, Medford, MA, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Daniel Killelea)

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**CONTROL ID:** 2228578

**CONTACT (NAME ONLY):** [Serena Carosso](#)

**TITLE:** [Progress toward the syntheses of novel monocyclic  \$\beta\$ -lactam antibiotics](#)

**ABSTRACT BODY:**

**Abstract:** The clinical introduction of penicillin in the 1940s is a milestone in the history of mankind since it led to a drastic decrease of the mortality rate caused by bacterial infections and also to an unprecedented improvement in the quality of life. The two decades between 1940 and 1960 have been defined as the “golden era of antibiotics” in which several new classes of antibiotics were developed and introduced on the market. However, infectious diseases have not been eradicated since bacteria progressively developed a wide variety of mechanisms to survive antibiotics, giving rise to the growing phenomenon of bacterial resistance. As a consequence the commonly used antibiotics are becoming less and less effective and the need for new antibiotics, with novel structures and/or mechanism of action, become every year more pressing.

My work in the Miller group deal with the development of new methodologies to be applied to the synthesis of monocyclic  $\beta$ -lactam antibiotics. In particular, we are interested in the synthesis of  $\beta$ -lactams which display a sulfur-containing side chain at the C4 position and an ATMO side chain at the C3 position. Several analogs have been generated through a synthetic route in which a bromine-induced cyclization is used for the construction of the  $\beta$ -lactam ring. The biological activity of the final compounds has been also evaluated.

Efforts have also been directed to the synthesis of monocyclic  $\beta$ -lactams containing an ATMO side chain at the C3 position and a 1,2,3-triazole moiety at the C4 position, which is introduced through the use of click chemistry. The biological activity of the final compounds will also be evaluated using in house agar diffusion essays.

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Rempex Pharmaceuticals -The Medicines Company, San Diego, CA, United States.  
2. Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2228425

**CONTACT (NAME ONLY):** [Krisanu Bandyopadhyay](#)

**TITLE:** [In situ generated metal nanoparticles as two-dimensional assemblies, core-shell structure and biosensor](#)

**ABSTRACT BODY:**

**Abstract:** Metallic and bi-metallic nanoparticles like gold, platinum, palladium, Au-Pt and Au-Pd of specific size immobilized on solid support has seen remarkable growth due to their different potential applications. Thus, there is a considerable interest for investigating a general preparative route to engineer aggregation-resistant metallic nanoparticles for various applications. The present study deals with *in situ* formation of two-dimensional assemblies of metallic and bi-metallic nanoparticles on functionalized surfaces. Electrochemical investigations of these nanoparticles revealed a highly efficient catalytic activity for many long-chain and poly alcohols including methanol, ethanol, 1-propanol, 2-propanol, ethylene glycol, and glycerol. In another application of this *in situ* metal nanoparticle synthesis, gold and palladium nanoshells have been synthesized successfully by reducing surface bound palladium and gold ions onto ~200 nm diameter silica core. The method for generating such nanoshells is based on seed-mediated growth technique. This present method reports the first time synthesis of palladium nanoshell from surface bound palladium nanoparticles seeds compare to earlier reports that use gold nanoparticles as seed to generate final palladium shell. In addition, the current study also involves synthesis of gold nanoshells on silica cores that are less than 100 nm diameter. Previous work has shown the successful synthesis of gold nanoshell on a ~200 nm silica core using the present seed mediated synthesis procedure. Gold nanoshells with a smaller core may find increased application in photo-thermal therapeutic studies. Finally, palladium nanoparticle assemblies generated on indium tin oxide (ITO) coated glass surfaces are applied towards detection of Dopamine (DA), an important neurotransmitter in the mammalian central nervous system. The sensing performance of the present biosensor is measured electrochemically using differential pulse voltammetry (DPV) and impedance spectroscopy, at different concentrations of dopamine in solution. The biosensor has shown a remarkably low detection limit for DA and a linear response over a wide concentration range. In addition, specificity of this biosensor for DA detection is also explored in presence of ascorbic acid (AA).

**ABSTRACT SYMPOSIUM NAME:** Research at Undergraduate Institutions - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Department of Natural Sciences , University of Michigan-Dearborn, Dearborn, MI, United States.

2. Department of Natural Sciences , University of Michigan-Dearborn , Dearborn , MI, United States.

3. Department of Natural Sciences , University of Michigan-Dearborn , Dearborn , MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Bradley Wile)

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**CONTROL ID:** 2228362

**CONTACT (NAME ONLY):** [Jun Li](#)

**TITLE:** [Self-cleaning surface by growing hierarchical ZnO nanowire coatings on micro-scale PMMA](#)

**ABSTRACT BODY:**

**Abstract:** In recent years, self-cleaning materials with lotus-effect, namely superhydrophobicity, and photocatalysis are attractive because of their eco-friendly characters. In this study, a hierarchical superhydrophobic and photocatalytic surface was constructed by growing various lengths of zinc oxide (ZnO) nanowires on micro-

scale polymethyl methacrylate (PMMA) surface that produced by electrostatic adherence and chemical etching. Firstly, the ZnO nanowires are applied as a coating onto PMMA substrates, and then silanization was used to offer enhanced water-repellence and hydrophobicity. At last, a hierarchical surface similar to lotus was obtained. The nano-size effect on wettability of nano/micro complex structures has been investigated by adjusting the ZnO nanowire length. As the nanowire length on the PMMA surface increases, a transition from the Wenzel state to the Cassie state occurs. A water contact angle as high as 155.7° was formed by growing ZnO nanowires of a suitable length on the micro-scale PMMA surface. Moreover, this material shows a high light transmission. Compression and impact experiments further demonstrate the robust superhydrophobicity of PMMA/ZnO nanowire hierarchical structures. The presented transparent materials offer an attractive alternative for surface treatments of glass, avoiding the use of environmental unfriendly chemicals.

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry and Sustainability - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Chemical Engineering, University of Michigan, Ann Arbor, MI, United States.  
2. Chemical Engineering, Harbin Institute of Technology, Harbin, Heilongjiang, China.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Sherine Obare)

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**CONTROL ID:** 2227756

**CONTACT (NAME ONLY):** [Jacqueline Arroyo](#)

**TITLE:** [Quantification of chromium in biological matrices](#)

**ABSTRACT BODY:**

**Abstract:** Chromium exposure happens in several ways, it is in the food and water we ingest, consumer products, and it is released by industrial activities. Measuring the exposure a person has had to a toxic element requires the sampling of tissues and fluids, such as those found in the ocular system. The human lens is of particular interest because it grows over an entire lifetime beginning from embryo and continuing through adulthood, therefore reflecting a lifetime of exposure. Chromium has two main oxidation states: trivalent and hexavalent, the trivalent form is necessary for glucose metabolism while the hexavalent form is toxic. The goal of this work is to develop a sample preparation protocol and method of analysis that can accurately quantify both states of chromium in biological matrices. Biological samples have a complex matrix that can include proteins, organic acids, and metals, all of which can effect the analysis. The current method uses cation exchange prior to the quantification of trivalent chromium by graphite furnace atomic absorption spectroscopy. Several studies designed to simulate the analysis of biological samples have been completed in order to evaluate the method's capabilities in four main criteria: interference of the sample matrix, limit of detection, specificity, and reproducibility.

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Loyola Univ, Chicago, IL, United States.  
2. Chemistry and Biochemistry, Loyola University of Chicago, Chicago, IL, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2227722

**CONTACT (NAME ONLY):** [Hollis Showalter](#)

**TITLE:** [A search for novel rifamycins and small molecule leads against \*M. tuberculosis\* RNA polymerase](#)

**ABSTRACT BODY:**

**Abstract:** Rifampin, a semisynthetic rifamycin, is the cornerstone of current tuberculosis treatment. Among many derivatives the benzoxazinorifamycins (bxRIFs), characterized by the clinical agent rifalazil, have great potential for tuberculosis (TB) treatment due to their superior affinity for wild-type and rifampin-resistant (Rif<sup>R</sup>) *Mycobacterium tuberculosis* RNA polymerases and their reduced hepatic Cyp450 induction activity. This presentation will detail x-ray crystal structures of *Escherichia coli* RNA polymerase complexed with two newer generation benzoxazinorifamycins. Consistent with our structure-based design approach, these structures show the C3'-tail of the benzoxazinorifamycin located in a gap between the  $\beta$  subunit fork loop 2 and  $\sigma$  finger of the polymerase. We will also discuss more recent work involving the development of an *in vitro* RNAP transcription assay that uses a fluorescent probe to detect transcription of RNA aptamers to the probe. This assay is being utilized in HTS against a clinically relevant Rif<sup>R</sup> RNAP mutant to search for novel inhibitory scaffolds. Preliminary results from the HTS will be discussed.

**ABSTRACT SYMPOSIUM NAME:** Parke-Davis, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Medicinal Chemistry, University of Michigan, Ann Arbor, Ann Arbor, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Mike Barbachyn)|Organizer (Jed Fisher)

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**CONTROL ID:** 2227569

**CONTACT (NAME ONLY):** [Kerry Rouhier](#)

**TITLE:** [A valine catabolic enzyme could be a potential target for altering the lipid or protein content in an oilseed](#)

**ABSTRACT BODY:**

**Abstract:** Seeds use storage reserves, such as lipids and protein, to fuel the early stages of germination, prior to the commencement of photosynthesis. These necessary reserves accumulate through various metabolic reactions during embryo development and seed maturation. One such reaction catalyzed by methylmalonate semialdehyde dehydrogenase (MMSDH) looks to play an important role in both lipid production and protein content in *Arabidopsis thaliana* seeds. MMSDH catalyzes an energy intensive step in valine catabolism by converting methylmalonate to propionyl-CoA (as well as malonate to acetyl-CoA). Recent results reveal decreased lipid and protein content in seeds lacking MMSDH. Other phenotypes such as seed viability, physical characteristics, and metabolic profiles also support its role in seed development. Based on these results, potential applications of an overexpression seed line could lead to seeds with increased lipid and protein content – something of interest to those seeking alternative biofuel mechanisms or food sources with altered protein content.

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Chemistry Department, Kenyon College, Gambier, OH, United States.  
2. University of Minnesota, Minneapolis, MN, United States.  
3. The JM Smucker Company, Orville, OH, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2223811

**CONTACT (NAME ONLY):** [Brian Stockman](#)

**TITLE:** [Nucleoside ribohydrolases as targets for \*Trichomonas vaginalis\* therapeutic agents](#)

**ABSTRACT BODY:**

**Abstract:** Trichomoniasis is the most prevalent non-viral sexually transmitted disease. Resistance to the 5-nitroimidazole class of therapeutic agents in use for the past 50 years has increased markedly, indicating the need for new therapies with novel mechanisms of action. *Trichomonas vaginalis* is an obligate parasite that relies on purine and pyrimidine salvage pathway enzymes to obtain its nucleobases. Nucleoside salvage pathway enzymes used by *T. vaginalis* are distinct from the pathway involved in activation of the 5-nitroimidazole drugs, and do not have mammalian counterparts, thus representing excellent targets for developing new antitrichomonal agents. The first step in this pathway is the hydrolysis of nucleosides to release the nucleobases. Uridine nucleoside ribohydrolase (UNH) and adenosine/guanosine preferring nucleoside ribohydrolase (AGNH) have been characterized and found to have distinct substrate specificities and thus recognize distinct pharmacophores. The druggability of the two enzymes was tested by developing an <sup>19</sup>F NMR-based activity assay to monitor the hydrolysis of 5-fluorouridine, and a <sup>1</sup>H NMR-based activity assay to monitor the hydrolysis of adenosine, and then screening the NIH Clinical Collection for inhibitors. Different classes of inhibitors were identified for the two enzymes confirming that they represent distinct, druggable targets. The best inhibitors were obtained commercially, structurally validated using 2D <sup>1</sup>H-<sup>13</sup>C NMR methods, and rank-ordered using IC<sub>50</sub> values determined by NMR. Suspected aggregators were also examined by assaying in the presence of detergent. Benzimidazole-containing proton-pump inhibitors were identified as μM inhibitors of UNH. Dipine-containing calcium channel blockers were also identified as UNH inhibitors, but these compounds were determined to be active in their phenylpyridine forms rather than the parent compounds. Flavonoid-based compounds were identified as μM inhibitors of AGNH. Active compounds are being further explored using a combination of activity assays, binding assays, fragmentation, and medicinal chemistry to define structure-activity relationships, as well as biological assays to correlate enzyme inhibition with antitrichomonal activity.

**ABSTRACT SYMPOSIUM NAME:** Upjohn, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Department of Chemistry, Adelphi University, Garden City, NY, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Jed Fisher)|Organizer (Mike Barbachyn)

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**CONTROL ID:** 2221483

**CONTACT (NAME ONLY):** [Ahmad Samin](#)

**TITLE:** [Synthesis and characterization of trimetallic Cu\(I\), Au\(I\) and Ag\(I\) complexes](#)

**ABSTRACT BODY:**

**Abstract:** The design and preparation of multinuclear metal complexes or coordination polymers containing direct metal-metal interactions, such as Pt-Ag, Pt-Tl, Pt-Pt, Pt-Pd, Au-Au, Ag-Ag, and Cu-Cu has received considerable attention. Among them, emissive copper(I) complexes are expected to be key materials for preparation of organic light emitting diodes likely because copper(I) is more cost-effective than the other precious metal complexes. In these systems metallophilicity plays an important role in assembling close M···M interactions.

Earlier our group reported the application of the 2-picoyl substituted NHC ligand toward stabilizing Ag(I)-Ag(I) interactions. The simple reaction of the NHC ligand precursor 1,3-bis(2-pyridinylmethyl)-1H-imidazolium tetrafluoroborate, [H(pyCH<sub>2</sub>)<sub>2</sub>im]BF<sub>4</sub> with silver oxide in acetonitrile produces the unusual triangulo-Ag<sub>3</sub> cluster, [Ag<sub>3</sub>(pyCH<sub>2</sub>)<sub>2</sub>im]<sub>3</sub>(BF<sub>4</sub>)<sub>3</sub>, with unusually short Ag-Ag separations (2.72 to 2.78 Å). We have now extended this chemistry to explore the electronic alteration of the ligand on the metal-metal separation. Additionally, we were able to produce mixed metal systems, and copper triangulo-Cu<sub>3</sub> clusters.

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

March 16, 2015 Joint Great Lakes and Central Regional Meeting (JGLCRM)

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Math and Science, American University of Afghanistan , Saint George, UT, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2220589

**CONTACT (NAME ONLY):** [Mohammad Rabbani](#)

**TITLE:** [Design and synthesis of nitrogen rich porous organic polymers](#)

**ABSTRACT BODY:**

**Abstract:** Recently porous organic polymers have been widely studied because of their multifunctionality. They have potential uses in areas such as storage, separation, and catalysis. It has been found that nitrogen rich porous organic polymers play significant roles in gas storage capacity and selectivity. We report here the synthesis of benzimidazole-linked polymers. Synthesized polymers are chemically and thermally stable due to the stability of benzimidazole moiety. Suitable building unit have been selected and synthesized to enrich the overall nitrogen heterogeneity in the frames. The polymers have moderate surface areas of around  $500 \text{ m}^2 \text{ g}^{-1}$ . Details synthesis and porous studies will be reported in poster presentation.

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Chemistry, University of Wisconsin-Platteville, Platteville, WI, United States.

2. Chemistry, University of Wisconsin-Platteville, Platteville, WI, United States.

3. Chemistry, University of Wisconsin-Platteville, Platteville, WI, United States.

4. Chemistry, University of Wisconsin-Platteville, Platteville, WI, United States.

5. Chemistry, University of Wisconsin-Platteville, Platteville, WI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2214639

**CONTACT (NAME ONLY):** [Matthew Mio](#)

**TITLE:** [Modified Sonogashira- and Glaser-type couplings: Reaction methodology for undergraduate research](#)

**ABSTRACT BODY:**

**Abstract:** Due to their structural rigidity, conjugation and unique bond torsion, sequence-specific arylethynylene and arylbutadiyne oligomers are excellent scaffolds for the study of shape-persistent supramolecular and nanoscale systems. With the ultimate goal of improving the generation of these important architectures, new synthetic methodologies have been developed utilizing an in situ ethynylsilane deprotection reaction. While synthetic strategies for the alkylation of aryl moieties (Sonogashira) or the homocoupling of alkynes (Glaser) traditionally involve iterative pathways, the use of an in situ ethynylsilane deprotection reaction has been shown to allow for the rapid construction, often in one pot, of complex arylethynylene and arylbutadiyne oligomers. Key to the protocol is the inclusion of a mixture of amidine base, such as 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU), CuI and substoichiometric amounts of water. The use of trimethylsilylacetylene versus bis-trimethylsilylacetylene, base toggling, inclusion of dioxygen for homocoupling, sterics of silylacetylene protection and CO insertion projects will be discussed.

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

March 16, 2015 Joint Great Lakes and Central Regional Meeting (JGLCRM)

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Chemistry and Biochemistry, University of Detroit Mercy, Berkley, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Jay Wackerly)

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**CONTROL ID:** 2213282

**CONTACT (NAME ONLY):** [Joong-Won Shin](#)

**TITLE:** [Vibrational spectroscopy of asparagine in acidic, neutral, and basic solutions](#)

**ABSTRACT BODY:**

**Abstract:** Fourier transform infrared spectroscopy (FTIR) utilizing attenuated total reflectance (ATR) was carried out to analyze changes in vibrational bands of asparagine (L-Asn) at 0.20 M concentration in acidic, neutral, and basic solutions in the pH range of 1 to 14. The spectra show evolution of peaks near 1730, 1680, 1260, and 1228  $\text{cm}^{-1}$  at pH values below 2, suggesting protonation of the carboxylic acid on the backbone of the molecule. The appearance of peaks near 1530, 1400, and 1360  $\text{cm}^{-1}$  at pH values in the 2 - 8 range implies that the amino acid adopts a zwitterionic structure.

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Division of Science, Governors State University, University Park, IL, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

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**CONTROL ID:** 2212323

**CONTACT (NAME ONLY):** [Jay Wackerly](#)

**TITLE:** [Synthesis and applications of oxaquinonacyclophane macrocycles](#)

**ABSTRACT BODY:**

**Abstract:** This presentation will feature research in our lab on the synthesis of a new class of redox active [1<sub>4</sub>]oxacyclophanes that contain *p*-benzoquinones. These macrocycles can be accessed in one-pot base catalyzed reactions of 2,3-dichloronaphthoquinone and various diphenols. Modifications to the electrophile and reactions conditions were also explored to access similar structures. Subsequently, each macrocycle was investigated for its ability to act as a supramolecular host for host-guest binding.

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Department of Chemistry, Central College, Pella, IA, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Jay Wackerly)

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**CONTROL ID:** 2211445

**CONTACT (NAME ONLY):** [Paul Cook](#)

**TITLE:** [X-ray crystallographic structure of BshC: A unique enzyme involved in bacillithiol biosynthesis](#)

**ABSTRACT BODY:**

**Abstract:** Bacillithiol is a low molecular weight thiol produced by many Gram-positive bacteria such as *Bacillus anthracis* and *Staphylococcus aureus*. The compound is involved in the maintenance of redox homeostasis and resistance to the FDA-approved antibiotic fosfomycin. It is produced via a pathway utilizing the enzymes BshA, BshB, and BshC. The structures and functions of enzymes similar to BshA (glycosyltransferase) and BshB (deacetylase) have been reported, but very little is known about BshC, the putative cysteine ligase in bacillithiol production. Here we report the first ever structure of BshC from *B. subtilis* to a resolution of 1.77 Å. The structure reveals that BshC contains a core Rossmann fold with extended connecting peptide motifs (CP1 and CP2) and an  $\alpha$ -helical coiled-coil domain that facilitates dimerization. The structure contains citrate and glycerol in the canonical active site and ADP in a second ligand binding site. The overall structure and bound ligands give insight into the function of this unique enzyme.

**ABSTRACT SYMPOSIUM NAME:** Mechanisms of Antibiotic Resistance - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Department of Chemistry, Grand Valley State University, Allendale, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Rachel Powers)

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**CONTROL ID:** 2211208

**CONTACT (NAME ONLY):** [Jennifer Batten](#)

**TITLE:** [Development and implementation of a summer camp for high school students based on the applications of analytical instrumentation in forensic chemistry](#)

**ABSTRACT BODY:**

**Abstract:** Chemistry in the real world is now permanently merged with technology and it is the goal of the Forensic Chemistry Summer Camps at Grand Rapids Community College to show area high school students how instrumentation is a key component in modern chemical analysis. The premise of the camps is that an arson crime (simulated) has been committed at an area college chemistry lab and it is the students' responsibility to analyze the crime scene evidence and identify a likely suspect. The students use procedures, which have elements of inquiry based discovery, to analyze ink, soil, accelerants, and DNA using UV-vis and atomic absorption spectroscopy, gas chromatography- mass spectrometry, and gel electrophoreses, respectively. This presentation will address the preparation, operation, and outcomes of the camps including the recruitment of student attendees, the laboratory investigations, and student feedback.

**ABSTRACT SYMPOSIUM NAME:** High School, Community College, and Undergraduate Education - Oral

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. Physical Sciences, Grand Rapids Community College, Jenison, MI, United States.

**DECISION STATUS:**

**SESSION HOST:** Organizer (Thomas Higgins)

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