

**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 constant 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 increase with the increasing temperatures. Forth, 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 the 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:**

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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:**

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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:**

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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:**

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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 pnicogen 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 pnicogen 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<sub>3</sub>N···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:**

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**CONTROL ID:** 2231227

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

**TITLE:** [Combined OM/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:**

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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:**

**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:**

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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:**

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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:**

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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:**

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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:**

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**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 ultraselective 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 ultraselective 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:**

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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 assays.

**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:**

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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:**

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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:**

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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:**

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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-base design approach, these structures show the C3'-tail of the benzoxazinorifamycin located in a gap between the β subunit fork loop 2 and σ 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:**

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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 x 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:**

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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-picoly 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,  $[H(pyCH_2)_2im]BF_4$  with silver oxide in acetonitrile produces the unusual triangulo-Ag<sub>3</sub> cluster,  $[Ag_3((pyCH_2)_2im)_3](BF_4)_3$ , 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

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

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

**DECISION STATUS:**

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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 m<sup>2</sup>g<sup>-1</sup>. 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:**

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

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

**DECISION STATUS:**

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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 cm<sup>-1</sup> 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 cm<sup>-1</sup> 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:**

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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]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:**

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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 α-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:**