

## **Characterization and Microstructural Analysis of High-Temperature Commercial Lead-Free Solder Alloys in Simulated Salt Spray Environment**

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The reliability of electronic assemblies is a hot topic. A device or package is only as strong as its weakest part, and the various solder joints that piece together an electronic assembly is often the part that fails the quickest. Thus, research has been conducted for a very long time on the properties of these solder joints and how to model their behavior, to be certain that they are suited for the application at hand. Up until recently the most popular solder to use in these assemblies was comprised of tin and lead (SnPb). This composition of solder was well understood, well modeled, and boasted favorable mechanical properties, making it ideal for almost all electronic applications. Unfortunately for this solder, lead has been phased out of the industry due to its negative health and environmental impact (as of 2007). This shift away from lead-based solder spurred a new line of research in the field of industrial systems engineering, as not only was there a search for a new alternative to SnPb solder, this new solder needed to be researched and understood enough to confidently use it in the applications where SnPb would have been used. Several new solder alloys have thus been studied (it is widely accepted that these new solders will be Sn-based, with other metal additions) however the most noteworthy of solders comes in the form of tin-silver-copper (SAC) and has proven itself time and time again to be a worthy successor to SnPb. Although certain compositions are more popular than others (Sn-3%Ag-0.5%Cu) and (Sn-4%Ag-0.5%Cu), there is no “one size fits all” composition that suits every application. Introducing even a small change to the composition of the solder can noticeably change how the solder behaves, making it very tunable for a particular addition. SAC based solder alloys are not in the clear yet; despite their universal acceptance there are still many questions concerning its reliability and performance under certain conditions. Being a more complex alloy than SnPb, much of its nuances and peculiarities, resulting in failure and other structural mechanisms, have not yet been truly modeled or accounted for. This is even further complicated when elemental or structural additions are added into the SAC composition. Additions such as bismuth, antimony, and nickel can affect how the microstructure of the solder is formed during the creation of the solder joint. Certain alloys of SAC utilize these extra metal additions in their solder, making them viable in applications where they will see constant use at higher temperatures, such as auto motives, aeronautics, and even naval craft. Such applications into vehicles and other crafts introduce a new performance variable that is often not accounted for; an aggressive saline corrosion environment. Whether it be an automotive that will experience saline corrosion via heavily salted roads during the winter time or marine vehicles being constantly exposed to salt water/salt spray, these applications are the most likely to experience this type of corrosion. The many elemental additions of these alloys can induce galvanic corrosion and excess chloride ions spur the creation of a passivation layer on the surface of the solder; the relative resistance to corrosion strongly relies on the solder’s ability to create a strong and protective passivation layer. The composition of the alloy directly correlates to the strength of this layer, and it is currently unknown how the many constituents of these multi-component SAC alloys will affect the creation of this protective layer. Since saline corrosion is electrochemical (galvanic) in nature, the addition of extra metals should change how the passivation layer is created and its relative strength. Although much research has been conducted on the mechanical properties of these high-temperature alloys in simulated working conditions, there has been no detailed experimentation concerning the effects of simulated saline corrosion on these specific alloys. Knowledge of corrosion mechanisms and its relationship to potential failure is key for utilization of these solder alloys in viable applications.

I’d like to thank the National Science Foundation (Award #1560390) for funding this research and allowing me to pursue this opportunity.

# Self assembly of fluorinated porphyrin monolayers on methylammoniumleadiodide perovskite surface

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Perovskite Solar Cells are a current topic of intense study, with methylammoniumleadiodide solar cells as one of the successful device architectures being pursued today. Organic solar cells have an efficiency near 11 percent whereas Hybrid Organic Inorganic Perovskites (HOIP) cells produce efficiencies up to 22 percent. However, their composition makes tailoring their electronic properties very difficult. The objective of this research is the interaction between applying free-based and metallated perfluorocarbon chained porphyrins to a perovskite surface in order to improve interfacial properties which increase work efficiency. This is made possible as fluorine atoms can attach to perovskite surface where we have examined this interaction via X-ray photoelectron spectroscopy (XPS), Kelvin probe microscopy (KPM), and Polarized modulated infrared reflection absorption spectroscopy (PMIRRAS). Free-based porphyrin along with Cobalt, Copper, Lead and Zinc metallated porphyrin were synthesized and examined. NSF award #1560390.

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## **Effects of GPER1 Activation on Progestin Receptor Gene Expression.**

**Ky'achia Rakell Joiray Atkins**

Gerald R. Hankins, Sabin Khadgi

There are several hypotheses that steroid sex hormones (progesterone and estrogen) have a role in suppressing cancer in males and females. Although there are several hypotheses, the pathobiology how sex hormones are involved in incidences of brain tumors is not completely known. Given the crosstalk between estrogen and progesterone signaling pathways, the objective of this research is to examine the effect of GPER1 activation on progestin receptor gene expression. U87 glioblastoma cells line were also used for this experiment as well. Glioblastoma is a malignant tumor affecting the brain or spine which arises from astrocytes in the central nervous system. The U87 cells were treated with GPER1 agonists (G1 and E2) and antagonists (G15 and G36). Given the inconsistencies of the Real Time RT-PCR for the cell line U87, we are continuing our research by running multiple PCR with different housekeeping gene (hRPS1-3) since the expression of the GAPDH appeared to vary with the treatments.

## Synthesis of New Thermosensitive Copolymers for the Modification of Polysaccharides

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The research of stimuli responsive polymers, also referred to as “smart polymers,” has recently become an area of interest for research. This is due to the polymers ability to undergo drastic change in physical properties in response to subtle changes in the environment such as temperature, salinity, pH, etc . One kind of smart polymer that has become particularly interesting are thermoresponsive polymers. These polymers are soluble at lower temperatures, however, self assemble into nangles at higher temperatures due to their lower critical solution temperature (LCST.) These nangles can be used to encapsulate hydrophobic drugs. It has been explored that the carbohydrate hyaluronic acid can be grafted to these polymers. This is beneficial since many cancerous macrophages use this as a fuel source and thus have receptors for it. This grafted polymer can specifically target these macrophages in a controlled manner. In this project we, explore different techniques to functionalize thermoresponsive polymers. The methods involve modifying the polymer in a way that will allow a coupling between the amine and carboxylic acid on hyaluronic acid. One method involved the modification of the of the thermosensitive RAFT polymer poly(diethylene glycol mono methyl methacrylate-co-butyl methacrylate) [poly(DEGMA-co-BMA)]. The end group of the polymer contains a thiocarbonylthio group which underwent an amine acid coupling with the the unprotected amine on boc ethylenediamine. This will result in the polymer containing an amine with the boc protecting group. We also explored the functionalization of the polymer poly(diethylene glycol acrylate-co-diacetone acrylamide) with adipic acid dihydrazide to add an amine onto the polymer. A polymer was synthesized via ring opening metathesis polymerization (ROMP.) We are exploring various terminating agents that contain a carboxyl group. The polymers were characterized via NMR, ultraviolet visible, and dynamic light scattering spectroscopy and fluorescence microscopy.

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The proliferation of non-small cell lung cancer cells is regulated by paraoxonase 2  
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**Abstract:** Non-small cell lung cancer (NSCLC) accounts for about 85% of lung cancer, which is the leading cause of cancer death in the world. High mortality rate associated with NSCLC is partially attributed to the limited understanding of NSCLC as well as ineffective therapeutic treatments. The initiation and progression of NSCLC involves genetic changes leading to alterations in the control of tissue development and homeostatic maintenance. Better knowledge about these genetic abnormalities is imperative for developing new chemotherapeutic drugs for NSCLC. Recent research demonstrates that the expression of paraoxonase 2 (PON2), a lactonase/arylesterase with anti-oxidant properties, are markedly enhanced in cancer tissues of NSCLC patients compared with corresponding adjacent non-tumorous tissues. Importantly, increased PON2 expression likely contributes to the resistance of NSCLC cells to classical anti-NSCLC therapeutic drugs. We found that stably reduced PON2 expression by siRNA reduced the proliferation of NSCLC cells but not their untransformed epithelia counterparts. To further elucidate the role of PON2 in NSCLC cell proliferation, we applied two newly developed gene-editing systems, TALEN and CRISPR/Cas, in the NSCLC cell line NCI-H1299. Our data indicated that Cas9 expression was induced by exogenous doxycycline in NSCLC cells in a reversible fashion. The goal of this study is to establish an efficient and scalable experimental approach interrupting the expression of a gene (e.g. PON2) in NSCLC cells, which provides a platform to investigate how changes in gene expression modulate NSCLC cell proliferation.

## Asymmetric Catalysis with Helical Supramolecular Polymers

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The objective of this research is to synthesize chiral helical polymers of benzene 1-monourea-3,5-bisamide (BUBA) monomers and coordinate them to copper. The capability of this copper catalyst to conduct enantioselective reactions will be tested in the hydrosilylation of prochiral aromatic ketones. It has been shown that helical polymers of benzene-1,3,5-tricarboxamide (BTA) can transfer chirality to a metal and display chiral amplification. BUBA monomers are easier to synthesize and may have different properties, so it is important to compare BUBA's self-assembly and properties to those of BTA.



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## Ambiphilic Compounds: Applications in Coordination Chemistry and Catalysis

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**Abstract:** The fundamental dative bonding of phosphorous' lone pair and boron's empty orbital has extended into a new topic of research in both coordination chemistry and catalysis. In recent years, the interest of Frustrated Lewis Pairs (FLPs) has evolved by experimenting ways to interrupt the natural interaction of phosphorus and boron. The Bourissou group has shown that these geometrically constrained Lewis pairs can work as transition metal ligands showing rare metal→borane interactions<sup>1</sup>. Another example of a unimolecular phosphorous-boron FLPs is Science published, D.W. Stephan's (C<sub>6</sub>H<sub>2</sub>Me<sub>3</sub>)<sub>2</sub>P(C<sub>6</sub>F<sub>4</sub>)B(C<sub>6</sub>F<sub>5</sub>)<sub>2</sub> showing that non-metallic PB combinations have the capability to activate and transfer H<sub>2</sub> such as transition metals<sup>2</sup>. Since then, several other PB compounds with varying organic linkers have been shown to activate small molecules such as dihydrogen under mild conditions. Our group has recently reported that a geometrically constrained FLP is an efficient catalyst in dehydrogenation of amine- and diamine-boranes<sup>3</sup>. This work aims at varying the spacer in phosphine-borane Lewis pairs in order to identify new FLPs that can be efficient in metal coordination and/or small molecule activation, targeting applications in TM and TM-free catalysis.

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# Novel Metal Phthalocyanine Nanowires for the Selective Detection of Toxic Gases in Highly Hydrated Environments

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## Abstract

In this project we synthesized metal phthalocyanines (MPcs) from Zn, Cu, Co, Ni, Fe and Mn using various approaches (solution reflux, solid state synthesis and solvothermal method). Utilizing chemical vapor deposition (CVD), we were able to grow MPc nanowires. These nanowires will be used for the selective detection of toxic gases at low concentrations. In our next steps, we propose to compare the detection limits of these MPc nanowires with those obtained from reactions of substituted MPcs with multi-fluorinated groups ( $-RF_5$ ) to follow the changes in their electrical conductivity and magnetic properties to help us develop gas sensors resistant to high percentages of humidity.

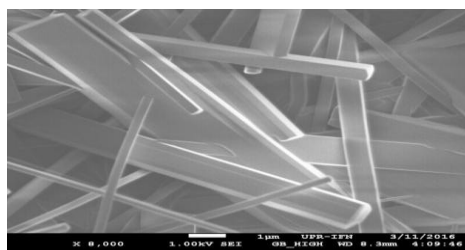


Figure 1 : SEM image of zinc phthalocyanine nanowires synthesized using CVD

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# Uncoordinated Cell Expansion Between Adjacent Cells Results in Cell Separation in the Moss *Physcomitrella patens*

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## Abstract:

One of the most important innovations of life on earth is the transition to multicellularity from unicellular ancestors, but little is known about barriers or drivers of this transition. Here we show that the control of multicellularity in the moss *Physcomitrella patens* is through PFT/PGGT-I and ROPs. PGGT-I (protein geranylgeranyltransferase-I) is composed of alpha and beta subunits, and all four ROPs in the moss *Physcomitrella patens* belong to type I ROPs, terminating with a canonical CaaL box, which is the PGGT-I target sequence. Previously, studies by the Bezanilla lab showed that transient knockdown of ROPs resulted in defects in cell adhesion and cell polarity, and studies by our lab have shown that knockouts of the *PpGGB* gene, which encodes for the geranylgeranyltransferase-I beta subunit, produces single-cell like plants. To systematically study the relationship of cell adhesion and the PGGT-I and ROP pathway, we have generated stable inducible knockdown lines of ROPs by artificial micro-RNA (amiRNA), which further confirmed the essential function of ROPs in cell adhesion and cell polarity. Moreover, while overexpression of ROP in the *ggb* mutant background rescued cell adhesion defects in *ggb* mutants, making the single-celled *ggb* plants form filamentous cells, overexpression of a mutant form of ROP, changing from CaaL to the non-prenylation target SaaL box, did not rescue. Similarly, while overexpression of ROP in the wild type background causes filamental protonemata to become round cells, overexpression of a mutant form ROP terminating with SaaL box did not affect any cell morphology. Using SEM and live imaging, we have found that the loss of cell adhesion is caused by uncontrolled and uncoordinated cell expansion, which could disrupt the cell walls. Thus, we propose that the PGGT-I and ROP pathway contributed to the evolution of multicellularity in plants by controlling coordinated cell expansion among neighboring cells.



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# **An Experimental Study on Heat Pipe Performance with Three-Dimensional Lattices Fabricated by Selective Laser Melting**

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## **Abstract:**

Overheating is a major concern in electronic devices and data centers as it directly affects its performance and reliability. Various cooling methods are implemented in the industry to solve this issue. Heat pipes are metallic tubes with porous structures that work based on phase change and capillary phenomenon. This heat transfer device allows the working fluid to travel through the porous structures against surface tension forces and without an external pump. In this research, metal heat pipes containing micron sized three-dimensional lattice structures, created by a computer aided design software, are fabricated by laser powder bed fusion. The process of powder bed fusion that is used is Selective Laser Melting, which melts metal in order for it to fuse and form 3D structures. These samples are being tested and compared with commercial heat pipes using an experimental setup. It is expected to see an enhancement in heat pipe performance by optimizing these additively manufactured structures.

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## Photoinduced trifluoromethylation of heterocycles

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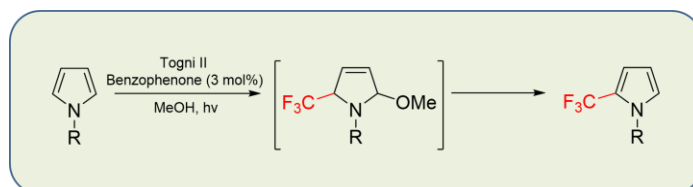
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### Abstract:

We present a mild, simple, and metal-free strategy for direct photochemical trifluoromethylation of heteroarenes. Preliminary work shows that a photoexcited state of benzophenone can function as an efficient radical initiator, readily generating trifluoromethyl radical from Togni II, a hypervalent iodine reagent. This reaction has been shown to tolerate a wide range of aromatic heterocyclic substrates, and research is currently being performed with the intent of broadening the scope to electron rich arenes and more complex molecules.

A dearomatized intermediate of this reaction has been isolated, and its structure elucidated with single-crystal X-ray diffraction. The substrate forms a bond with a molecule of the solvent alcohol, suggesting that interesting intramolecular chemistry may be possible. The intermediate contains an olefin moiety, and we envisage the application of stereoselective functionalization methods toward the synthesis of complex molecular products.





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# **Resorufin characterization and optimization of pulsed excitation system in electrochemistry-coupled fluorescence microscope**

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## **Abstract:**

Studying the effects of electrochemistry on the fluorescence signals of different molecules has proved to be a promising new characterization technique with applications in a variety of fields <sup>[1]</sup>. A microscopy set-up that combines an electrochemical cell with a fluorescence microscope has been successfully used to study molecules that exhibit a reversible switch of emission by controlling their redox state <sup>[2,3]</sup>. The coupled microscope has an epifluorescence set-up with a white light continuous excitation system. This set-up has been successful in the characterization of tetrazine dyes, but the study of a water-soluble dye is necessary for future studies of biological systems. Furthermore, is it possible to create a new optical set-up that uses a pulsed LED as the source of illumination. This would allow for the measurement of fluorescent lifetimes in a sample. This study focuses on both the characterization of a water-soluble molecule (resorufin) and the optimization of the new pulsed excitation system. This first objective is achieved by measuring resorufin's fluorescence under different electrochemical parameters; the second objective is investigated by experimental measurements of the illumination profiles of both the current and new excitation systems. Preliminary results show that resorufin appears to be a good candidate as a redox mediator and fluorescent reporter for future studies, and that the new proposed illumination set-up has slightly improved the illumination profile of pulsed LED excitation while maintaining the continuous excitation capabilities. However, further modifications to optimize the pulsed excitation system will be conducted and analyzed through lifetime measurements.

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# **Development of a microscopy system for studying ultrafast transient optical properties of gold nanoparticles**

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## **Affiliations**

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**Abstract:** Incident light on gold nanoparticles (AuNPs) causes the conduction electrons to oscillate. Resonance of this oscillation due to excitation of AuNPs at a characteristic frequency is referred to as localized surface plasmon resonance (LSPR). Excitation of AuNPs at LSPR frequencies leads to efficient conversion of light into heat and strongly enhanced electromagnetic waves in the near field regime. Also, excitation of AuNPs at LSPR frequencies with an ultrashort laser pulse causes ejection of electrons from the AuNPs. Additionally, the LSPR strongly depends on the shape and size of the AuNP and on the dielectric properties of the surrounding medium and can be tuned to the window of maximum transparency of biological tissues. As such, AuNPs promise to have applications in areas such as biological sensing and cancer therapies. The transient response of AuNPs to ultrafast laser pulses can be studied using pump-probe spectroscopy. Unfortunately, small sample sizes often make AuNPs difficult to study. This issue can be alleviated by coupling a pump-probe spectroscopy system to a microscope. My ongoing research focuses on the development and installation of a pump-probe microscopy system. In addition, the design should also allow coupling with a normal spectrometer.



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## **Development of Multimodal antimicrobial drugs targeting the inhibition of the Methylerythritol Phosphate (MEP) Pathway**

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**Abstract:** The MEP pathway is essential for the synthesis of the two isoprenoid precursors isopentenyl diphosphate (IPP) and dimethylallyl diphosphate (DMAPP) in many pathogenic microbes. Its absence in humans lends itself as an ideal target for the development of new anti-microbial drugs to counter drug resistant pathogens. Particular interest lies in the precursor (*E*)-1-hydroxy-2-methyl-2-butenyl-4-diphosphate (HMB-PP) which is converted to IPP and DMAPP via the enzyme IspH. HMB-PP is an effective natural phosphoantigen for activating V $\gamma$ 9V $\delta$ 2 T-cells, while analogs of HMB-PP have been shown to effectively inhibit the IspH enzyme. The goal of this project is to mask the polar phosphate group of these small molecules with a prodrug moiety to bypass the nonpolar cell membranes. Once synthesized, *in vitro* tests on V $\gamma$ 9V $\delta$ 2 T-cells and variety of pathogenic bacteria such as *Escherichia coli* will be used to determine the drug's effectiveness.

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M. Davey *Med. Chem.* (2018), 61, 2111–2117

## Generation of Solid-State, Efficient Emitters Based on 6-Membered Ring Excited State Intramolecular Proton Transfer (ESPIT) Systems.

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The synthesis of benzimidazole based molecules have shown to have peculiar optical properties through Excited State Intramolecular Proton Transfer (ESPIT) mechanisms. These molecules' fluorescence depend on a prototropy from an Enol (E) to a Keto (K) state, after photon absorption. This tautomeric shift renders a large red-shifted emission, an increased sensitivity to environmental polarity, and occasionally double fluorescence. These properties can be exploited to produce ratiometric probes in both solution and in solid-state. *Ab initio* calculations have shown similar quantum yields for both states, unlike previously studied organic fluorophores.<sup>[1]</sup> Application of these novel probes could be implemented in biologic processes, environmental pollutant sensing, and safety inks.

Project Mentor: Professor Antoinette De Nicola, Department of Chemistry

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## **Understanding the Fate of Products After Reactivation of Acetylcholinesterase with QM/MM Simulations**

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### **Abstract:**

Acetylcholinesterase (AChE) is an enzyme involved in the hydrolysis of the neurotransmitter acetylcholine (ACh). Regulation of ACh by AChE is necessary for optimal signal transmission between neurons and thus the inhibition of AChE leads to an overactivation of synapses with resulting neurological symptoms including death. Organophosphates (OPs) are a class of molecules known as AChE inhibitors which bind covalently and irreversibly to the serine residue in the catalytic triad of the active site of AChE and render the enzyme inactive. Despite their lethality in small doses and their ability to serve as nerve agents, OPs are still widely used as pesticides and chronic exposure poses a major threat to public health. The study of oximes, a group of nitrogen-containing organic compounds known for their ability to reactivate and restore AChE, is therefore of clear and vital interest. Using quantum mechanical (QM) and molecular mechanical (MM) calculations, we plan to study the degradation of oximes after reactivation in order to gain a better understanding of the oxime reactivation mechanism and of the environment of the AChE active site. Early data from QM simulations indicate that oxime degradation requires the presence of solvent. Discoveries in this field may contribute to advancements in the design of therapeutic compounds against OP poisoning.

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# Photocatalytic Degradation of Waste Water Pollutants- Impact of TiO<sub>2</sub> Phase on the Decomposition of Lactic Acid

*Annika, Holm*

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Chantal Guillard, Université de Lyon, Institut de Recherches sur la Catalyse et l'Environnement de Lyon, UMR 5256, CNRS, Université Claude Bernard Lyon 1, 2 avenue A. Einstein, F-69626, Villeurbanne, France

## Abstract

Titanium Dioxide-based photocatalysts have been well studied because of their ability to facilitate the oxidation of waste water and air pollutant molecules in the presence of UV light. TiO<sub>2</sub> exists in two main phases: anatase and rutile. Lactic acid is particularly interesting as a model pollutant because of its abundance in agricultural and agro-industrial waste. It can be produced chemically, or by the process of fermentation. Anatase and anatase/rutile composites are generally the most efficient, and more commonly used for industrial and commercial purposes. However, the improvement of rutile TiO<sub>2</sub>'s efficiency could be interesting due to its ability to absorb a large amount of solar light. The goal of our group is to study several types of titanium dioxide, and understand how the structural and textural properties of each material affects its efficiency. We also hope to establish the degradation pathways of lactic acid, and how TiO<sub>2</sub>'s properties might play a role in this.

NSF award #1560390



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## **A PAPER-BASED MICROFLUIDIC PLATFORM FOR PHOTOSYNTHETIC BIOELECTRICITY GENERATION**

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Bioelectronics & Microsystems Laboratory, Department of Electrical & Computer Engineering,  
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Paper-based devices have recently emerged as simple and low-cost paradigms for fluid manipulation and analytical/clinical testing. However, there are significant challenges in developing paper-based devices at the system level, which contain integrated paper-based power sources. We aimed to develop a simple, inexpensive, disposable paper-based microfluidic device for self-sustaining bioelectricity generation through microbial photosynthesis. We developed a paper-based bio-solar cell generating a current density of  $58 \mu\text{A}/\text{cm}^2$  and a power density of  $4 \mu\text{W}/\text{cm}^2$ , these are comparable to or higher than values for micro-sized biosolar cells and other paper-based bacteria-powered batteries. This paper-based microfluidic platform features significant performance enhancement by (i) maximizing solar energy capture with a transparent sealing layer, (ii) reducing cathodic overpotential with a solid-state cathode and (iii) constructing a highly conductive and hydrophilic reservoir. The microliter-scale paper device with photosynthetic bacteria generated self-sustained electricity for more than 3 hours. This presented device is the first paper-based bio-solar cell that could facilitate high power density and energy efficiency with self-sustainability. We hope that with each rendition of this battery the power density and energy efficiency will improve. As of now, one of these devices can only power equivalent to an LED light bulb for 20 minutes, but, small devices like this could one day replace oil, coal, or even solar energy.



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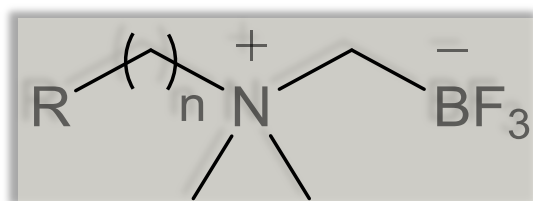


## Zwitterionic Alkylammoniummethytrifluoroborates (AMBF<sub>3</sub>) for <sup>18</sup>F PET Imaging

Stephanie León Quiñonez, Dr. Emmanuel Gras, Dr. James Sacchettini

LCC CNRS and Texas A&M University

**Abstract:** To develop new ways to target diseases, it is essential to monitor *in vivo* molecular events for a detailed picture of metabolic processes. Positron Emission Tomography (PET) is a non-invasive molecular imaging technique that uses positron emitting radiopharmaceuticals.<sup>1</sup> A drawback of PET is the short activity of its positron-emitting isotopes, where <sup>18</sup>F has the most appropriate half-life ( $t_{1/2}$  = 110 min), contributing to its wide utility.<sup>2</sup> Given the loss of F<sup>-</sup> nucleophilicity in water, which causes the addition of extra steps in the synthesis of bioconjugatable probes and thus decreases their useful imaging time frame, new probes stable in aqueous media are needed.<sup>3</sup> Ammoniomethyltrifluoroborates (AMBF<sub>3</sub>) can undergo a one-step <sup>18</sup>F-<sup>19</sup>F isotope exchange (IEX) under aqueous conditions with the zwitterionic property further enhancing its aqueous stability.<sup>4</sup> This research aims to synthesize zwitterionic AMBF<sub>3</sub> probes with varying linker length to increase their bioconjugability and stability. An AMBF<sub>3</sub> probe (n = 3) was synthesized and needs purification and consequent biomolecular analyses and functionalization for further development.



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# A Novel Method for Simulating Diffracted Light

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## Diagram of Theoretical Experiment



## Abstract

This research project shows a new method for simulating diffracted light by theoretically decomposing light into Hermite-Gaussian (HG) modes. Using the electric field amplitude of HG modes, an orthonormal condition was derived analytically and verified computationally. Then, intensity profiles of HG modes were simulated from lower-order to higher-order. By calculating the coefficients of different HG modes, we were able to simulate the diffracted field intensity of a laser beam after it leaves a rectangular aperture. In the simulation, the intensity profiles depict near field, intermediate field, and far field diffraction patterns. The far field results calculated using Kirchoff's diffraction formula are consistent with the results of this project; thus, this novel theory is validated.

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# **Simulation of the Electronic Properties of Group 14 Phthalocyanine Derivatives**

**A.Nkansah<sup>12</sup>, F. Castet<sup>1</sup>, S. M. Gali<sup>1</sup>, B.H. Lessard<sup>4</sup>, Luca Muccioli<sup>3</sup>, Chad Risko<sup>2</sup>**

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**2 Department of Chemistry, University of Kentucky, Lexington, USA;**

**3 Department of Industrial Chemistry, University of Bologna, Bologna, Italy;**

**4 University of Ottawa, Department of Chemical Engineering, Ontario, Canada**

**Abstract:** The focus of this project is to apply computational materials chemistry approaches to understand the ambipolarity of charge transport in crystalline Group 14 phthalocyanines. Such molecular materials, which fall under the broader context of organic semiconductors, are of interest for next generation, flexible electronics applications. More specifically, the project will deploy theoretical simulations run in a high-performance computing environment to provide evidence that the dimensionality of charge transport in these materials can be finely tuned by substituting the phenoxy axial groups with fluorine atoms and by varying their number of positions. In this step of the data collection process the theoretical simulations were used to compute the energy values for different variations of phthalocyanine, internal reorganization energies, Huang-Rhys parameters for hole transport, and the shapes of the molecular orbitals.

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# **High-Field NMR Spectroscopy and Mass Spectrometry for the Quality Control of *Epimedium Grandiflorum* Herbal Supplements**

**Ifunanya Okeke (supervisor: Myriam Malet-Martino)**

**Paul Sabatier University, Scripps College**

*Epimedium grandiflorum* has an extensive history in traditional Chinese medicine, and as a commercially-available herbal supplement used to treat a myriad of ailments. However, the prevalence of poor-quality supplements has made determining the composition of active ingredients in marketed *Epimedium* herbal supplements a shared interest between marketers and researchers alike. Herein, high-field  $^1\text{H}$  NMR spectroscopy and electrospray ionization mass spectroscopy in positive mode (ESI+ MS) are used in an attempt to identify biologically active molecules in two commercial herbal supplements of *E. grandiflorum*. Nine prenylflavonoid glycosidic compounds were initially chosen as possible constituents of these two supplements. Their identities were confirmed using the stated techniques before further analysis. Preliminary results revealed that one standard, baohuoside V, was incorrectly manufactured. Thus, it was excluded from further studies. Subsequent ESI+ MS and MS/MS analysis confirmed the presence of the remaining eight standards in the supplements.

Due to the similar structures of the prenylflavonoid glycosidic compounds found in *Epimedium grandiflorum*, it was difficult to fully determine their identities and quantify their amounts within the two herbal supplements based solely on 1D  $^1\text{H}$  NMR technique. These problems will be approached in future studies, utilizing homonuclear correlation spectroscopy (COSY), heteronuclear single quantum coherence (HSQC) and heteronuclear multiple bond correlation (HMBC) NMR experiments. From here, experimental quantities can be compared against those stated by manufacturers, thus continuing the work of quality control.



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## **Micro-mirrors for Microfluidic Ray Optics**

**Claire Onsager, Jean Frederic Audibert, Dr. Robert Pansu**

**University of Michigan, École normale supérieure Paris-Saclay, Institut d'Alembert**

### **Abstract:**

In an effort to obtain more perspectives of a sample under a microscope, it is necessary to fabricate micro-mirrors to place over a capillary tube. It is hoped to obtain this with use of an Ultimaker 2+ 3D printer and the design program Google Sketch UP. The challenge is to 3D print a small curved surface that is also optically clean. Then, modification of the Tollens process will be used to coat the surface in silver.

*Scheme legend.*

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# Direct Laser Writing of 3D Magneto-Photonic Microstructures for Biomedical Applications

PERRY Amber, AU Thi Huong, LAI Ngoc Diep

Laboratoire de Photonique Quantique et Moléculaire

**Abstract:** *The coupling of photonic structures with bi-model fluorescence and magnetic properties is a topic of great interest in the research community. Our work explores the coupling of a single photon source based on a colloidal semiconductor nanocrystal (NC), also known as a colloidal quantum dot (QD), into a polymer-based photonic structure doped with magnetic nanoparticles. We use the low one-photon absorption (LOPA) direct laser writing (DLW) technique to fabricate 2D and 3D SU-8 microstructures doped with magnetic nanoparticles and containing a single embedded CdSe/CdS NC, while keeping the NC's single photon source properties.<sup>1</sup> An external magnetic field is applied to manipulate the movement of the microstructures containing fluorescence emitted from the QDs. We can then perform fluorescent checking to track the movement of the QDs. This project contributes to a wide range of applications in quantum information processing, quantum dot-based solid-state platforms, biolabeling, and more.*

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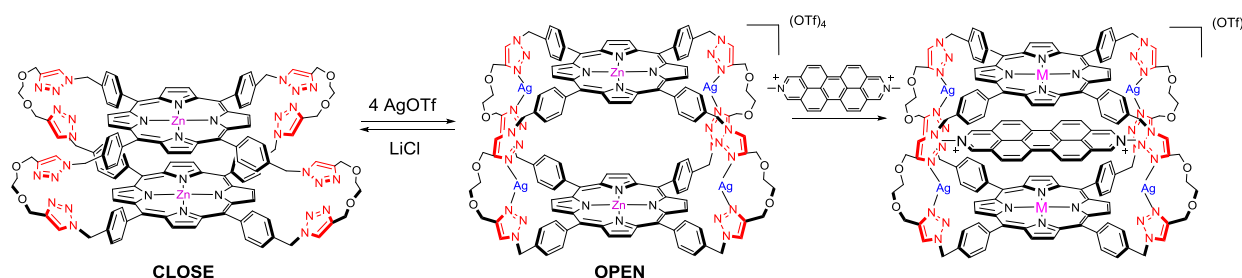
# Synthesis of Diazaperopyrenium Dication as Guest in a Switchable Molecular Cage

Zari M. Preyer,<sup>1</sup> Henri-Pierre Jacquot de Rouville,<sup>1</sup>  
Ryan Djemili,<sup>1</sup> Stéphanie Durot,<sup>1</sup> Valérie Heitz<sup>1</sup>

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67000 Strasbourg, France > Email: [v.heitz@unistra.fr](mailto:v.heitz@unistra.fr)

## Abstract:

Supramolecular chemistry can be defined as the chemistry behind the molecule.<sup>[1]</sup> In this field, molecules are assembled by noncovalent interactions (H-bonding,  $\pi$ - $\pi$ , Van der Waals, etc.) to form more complex structures. Among these structures, molecular cages are 3D hollow structures which have the feature to encapsulate molecules in their cavity.<sup>[2]</sup> However, examples of cage-type compounds able to modulate their cavity sizes are still limited. A *bis*-porphyrin cage incorporating triazolyl ligands have been developed as a switchable receptor.<sup>[3]</sup> Upon addition of metallic centers (Ag (I)), the cavity size formed by the two porphyrins can be opened to permit the inclusion of guest molecules by  $\pi$ - $\pi$  stacking interactions (Figure 1). Here, we focus on the synthesis of diazaperopyrenium dication<sup>[4]</sup> as a promising guest candidate (large electro-deficient molecule) for its encapsulation inside the cage.



**Figure 1.** Upon addition silver(I) ions, expansion of the bis-porphyrin cage allows the incorporation of an electro-deficient aromatic guest.

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## **An Ecological Study of the Chemical Composition and Identification of Indigenous Microorganisms of Schenectady's Vale Park and Cemetery.**

Hafsah Zorqane, Elizabeth Rivera\*, Stafford Bowman, Alycia Boodhan, Matthew Helms, Madison Montanye, Lorena Harris PhD and Richard Simons PhD

SUNY Schenectady County Community College

**Host Institution:** The University of Toulouse

### **Abstract**

Vale Cemetery and Park is established in 1857 is a recreational area in Schenectady, NY where SUNY Schenectady County Community College and LSAMP students observed, performed and developed a research exploration of the aquatic ecology. Our purpose was to identify microbial organisms in the water, changes in population size, seasonal activity, and characterization of the chemical composition of the water reservoirs of the park. Identification of the genus of ten microorganisms was performed using tests including chemical, biochemical and microbiological techniques. Seven different genera among the ten individual microbes were identified as *Klebsiella spp*; *Micrococcus spp*; *Neisseria spp*; *Roultella spp*; *Staphylococcus spp*; *Streptomyces spp*; *Streptococcus spp*; and molecular techniques are being performed to determine the specific species, through amplification and sequencing of the rRNA conserved gene of these microbes. In addition, chemical tests, including pH, hardness, iron, chloride, among others, were conducted in numerous trials to establish the environmental conditions in which the microbes identified are contained, thus allowing us to contribute to the park's chemical composition and safety awareness. The Vale Park educational research program from SUNY SCCC in cooperation with park management could be a model for aspiring researchers at community colleges to increase a sense of belonging to the broader community and awareness of the local environment.



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# DIRECT LASER WRITING OF METALLIC NANOSTRUCTURES: APPLICATION TO DATA STORAGE AND COLOR NANOPRINTING

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Laboratoire de Photonique Quantique et Moléculaire

**Abstract:** *Due to plasmonic effects, light interacts with free electrons of nanoparticles to create induced dipoles which cause absorption of light of varying wavelengths. By changing the size of the nanoparticles, we are able to change the spectrum of absorption of the nanoparticles. Focusing a laser beam to a small focal point causes a local hot spot to occur at the focal point. When this local hot spot is set on a thin film of metal, the intense heat causes the dewetting effect to occur. The dewetting effect causes the thin film of metal to form nanoparticles that are of size on the order of tens of nanometers. By changing the power of the beam incident on the film and the speed at which the beam moves over the film, we are able to vary the size of the nanoparticles and thus vary the absorption spectrum of the nanoparticles. In our work, we are attempting to realize structures, such as text or images, on the scale of a few microns that are made of constituent nanoparticles with varying absorption and emission spectrums. In previous work, the realization of these structures has been achieved on gold, while we are focusing on the use of aluminum and silver.*

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# **Cells Mechanotransduction: Geometrical Confinement for cell wave control**

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3. Mechanical Engineering Department, California State University, Fullerton

Organisms develop from a single cell through a complicated procedure with multiple factors. One of the factors that decide a role of a cell in an organism is the spatial patterning of cell behavior. Cells travel in a mechanical wave like pattern with a certain wave length. We investigate the characteristics of the mechanical waves by confining tissues to a certain geometry that interferes with the wave length of the cell, manipulate the environment of the cell, then analyze the tissue reaction using Particle Image Velocimetry (PIV) and Traction Force Microscopy (TFM).

NSF AWARD #1560390

NSF grant # 1302873

Title: Formation and studies of spin crossover complex molecular films

Name: Xavier Thompson

Advisors: Drs. Lucie Routaboul and Scott Williams

Director of Group: Dr. Azzedine Bousseksou

Team Members: Dr. Gabor Molnar, Dr. Lionel Salmon, Dr. William Nicolazzi, Lea Gogard, Dr. Victoria Shalabaeva, Dr. Karl Ridier, Alin-Ciprian Bas, José Elias Angulo Cervera, Mario Piedrahita Bello, Ahlem Regradj, Ayman Kanaan, Florian Meunier

NSF award: #1560390, UPR CNRS 8241

Abstract:

The laboratory of Coordination Chemistry is a CNRS funded laboratory in Toulouse, France with three themes: health, materials and catalysis. The laboratory focuses on coordination chemistry to advance these fields and Team P specifically focuses on spin crossover complexes, a class of smart molecules with switching capability at the solid state. Spin Crossover (SCO) materials exhibit a reversible change from low spin to high spin with the application of an external stimulus. The spin transition triggers a change in their physico-chemical properties as volume, color, and magnetic properties. These changes are promising mechanisms to help develop nanoelectronics such as molecular switches, actuators, and sensors. The subject of my training is to form and study molecular spin crossover films on different substrates. The goal of my project is to form high quality films that are strongly anchored on the substrate, which is needed for applications.

# The application of (2-Hydroxyethyl Methacrylate) HEMA hydrogel for wound healing.

*Zoe Vaughn*

Joseph A Gardella Jr., Buffalo NY & University at Buffalo (USA)

## Abstract

Chronic wound care has been gaining momentum due to drug delivery with the use of growth factors. Proteins such as Keratinocyte Growth Factor, KGF, leads to wound healing in the epithelial cells and KGF has proven to promote wound closure. Hydrogels, water swollen structures composed mainly of hydrophilic homopolymers or copolymers, serve as a vehicle that delivers the desired substance into the exact location needed for wound healing.

Hydrogels aqueous nature allows the material to accommodate various therapeutic factors. 2-Hydroxyethyl Methacrylate, HEMA, hydrogel is used because of its ability to achieve different characteristics without much change to the polymer. Through swelling of HEMA and perfluoropolyether, PFPE, the barrier layer, it was proven that HEMA holds up to 60% water by weight. Through the study it shows that HEMA is an optimal hydrogel to use when up taking a protein. Also HEMA, has the ability to uptake KGF, proven through the results of the controlled release study. Knowledge that KGF is up taken was further proved by fluorescence and TOF SIMS. Uptake and release studies conducted on Green Fluorescence Protein, GFP, a reporter gene, proved that HEMA can uptake protein. Studies that crosslinked methyl methacrylate, MMA with HEMA and methylacrylic acid, MAA with HEMA were conducted to increase the water content that the hydrogel could hold. This would result in a more stable environment for the protein KGF to be uptaken and released in.

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# Design of Protein Mimetics by Dynamic Combinatorial Chemistry on Folded Peptidic Scaffolds

**Gabrielle Webb, Taleen Peker, Benjamin Zagiel, Roba Moumné,  
Ph.D**

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University of Florida iREU

**Abstract:** *(Keep it short – you should not exceed one page overall)*

Peptide mimetics is an attractive method to identify potential binding partners for otherwise difficult targets<sup>1</sup>. These smaller versions of proteins are easier to manipulate and optimize over larger more traditional pharmaceutical compounds. To produce easily exchangeable peptides, the group utilizes dynamic combinatorial chemistry (DCC) to create a library of peptides, adorned with switchable building blocks for functionalization. When the library is introduced to a target, the library progresses to the target-building block configuration that is the most stable while leaving the rest of the building blocks in solution<sup>2</sup>. We use cysteines as connectors between the peptide scaffold and the building blocks. For these studies to be successful, information about the scaffolds and every single building block to be included in the library must be collected. Multiple DCC experiments were performed with varying levels of complex libraries, composed of scaffolds and building blocks. HPLC, MALDI TOF mass spectrometry, and NMR were used to verify the purity and identity of these peptide scaffolds. Progress of these reactions were analyzed using analytical HPLC. The products were all identified on analytical HPLC based on the retention times of pure BBs and scaffolds as well as mass spectrometry.

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