The Seventh Annual
Undergraduate Research Symposium

Sponsored by the Western New York Section
of the American Chemical Society

Saturday April 19, 2014
University at Buffalo, SUNY
Welcome Message From The Organizing Committee

Welcome to the 7th annual Undergraduate Research Symposium sponsored by the Western New York Section of the American Chemical Society! This Symposium highlights some of the exciting research being performed by exceptional undergraduates and their mentors from a variety of institutions throughout western New York and the surrounding areas, including southern Ontario.

We hope all participants will feel free to engage one another in active discussions about the stimulating science being presented. Please use this meeting as an opportunity to develop professionally by networking with scientific peers and faculty mentors in a relaxed scientific atmosphere.

A big ‘Thank You’ to all of our 35 student presenters and especially to our keynote speaker, Prof. Krista Walton, of the Georgia Institute of Technology. I would also like to extend my appreciation to our generous sponsors and to the members of the Organizing Committee, without whom this Symposium would not be possible.

Sincerely,

Jason Benedict
Chair, 2014 Symposium Committee

2014 Symposium Organizing Committee

Chair: Dr. Jason B. Benedict
Department of Chemistry, University at Buffalo, SUNY

Dr. Timothy M. Gregg
Department of Chemistry and Biochemistry, Canisius College

Dr. Sarbajit Banerjee
Dr. Valerie A. Frerichs
Dr. Andrew Murkin
Dr. Javid Rzayev
Dr. Luis Velarde
Department of Chemistry, University at Buffalo SUNY

Dr. Robyn Goacher
Department of Biochemistry, Chemistry and Physics, Niagara University
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Our Keynote Speaker

Krista S. Walton holds a B.S.E in Chemical Engineering from the University of Alabama-Huntsville (2000) and PhD in Chemical Engineering from Vanderbilt University (2005). She completed an ACS PRF Postdoctoral Fellowship at Northwestern University under the supervision of Prof. Randall Snurr and joined the faculty at Kansas State University in 2006 as an assistant professor. Dr. Walton moved to the School of Chemical & Biomolecular Engineering at the Georgia Institute of Technology in 2009 and currently holds the position of Associate Professor and Marvin R. McClatchey and Ruth McClatchey Cline Faculty Fellow. She has won several awards including the Presidential Early Career Award for Scientists and Engineering (PECASE), NSF CAREER Award, Army Research Office Young Investigator Award, and the inaugural 2013 International Adsorption Society Award for Excellence in Publications. Dr. Walton’s research group focuses broadly on the design and synthesis of next-generation multifunctional, porous materials with molecule-specific properties for adsorption applications including adsorption separations, air purification, carbon dioxide capture, chemical sensing, and catalysis.
Schedule of Events
April 19, 2014
Natural Sciences Complex (NSC) North Campus, University at Buffalo

9:00 am-9:50 am    Registration
9:50 am-10:00 am   Introductory Remarks: Prof. Timothy Gregg and Prof. Jason Benedict
10:00 am-10:50 am  Keynote: Prof. Krista Walton, Georgia Institute of Technology.
                   “Synthesis and Application of Porous Inorganic-Organic Hybrids”
11:00 am-12:30 pm  Student Oral Presentations: Moderator Prof. Luis Velarde
                   Eoghan Connors, SUNY College of Env. Science and Forestry
                   Umar Asif, St. Bonaventure University
                   Jason Biasini, SUNY Oswego
                   Jennifer Yoon, Syracuse University
                   Daniel Stuart, McMaster University
                   Carly Rolph, Hobart and William Smith College
12:00 pm-12:15 pm  Lunch (NSC-216)
12:15 pm-12:30 pm  Poster Presentations (Hallway near Mrs. Richs)
12:30 pm-1:30 pm   Symposium Awards and Closing remarks: Prof. Jason Benedict
Oral Presentations
Time: 10:00 AM - 12:30 PM  (NSC room 215)

Keynote Address
10:00 am Krista S. Walton, Ph.D. Georgia Institute of Technology
Synthesis and Application of Porous Inorganic-Organic Hybrids

Student Presentations

1. 11:00 am Eoghan L. Connors SUNY College of Env. Science and Forestry
"Green" Synthesis of Compounds with Biomedical Significance Facilitated by Water-Soluble Dendritic-Palladium Complexes

2. 11:15 am Umar Asif St. Bonaventure University
Synthesis of Biaryl Precursors for the Bottom-Up Fabrication of Graphene Nanoribbons

3. 11:30 am Jason Biasini SUNY Oswego
Microwave-Assisted Synthesis of Thiazolidinedione Compound Library

4. 11:45 am Jennifer H. Yoon Syracuse University
Allosterically Regulated Catalyst of Retroaldol Reaction

5. 12:00 am Daniel Stuart McMaster University
\([\text{XeF}_5]^+\) and \([\text{Xe}_2\text{F}_{10}]^+\) Salts of the \([\text{Cr}^\text{IV}\text{F}_6]^{2-}\), \([\text{Cr}^\text{V}\text{OF}_3]^{2-}\), and \([\text{Cr}^\text{V}_3\text{O}_2\text{F}_8]^{2-}\) Anions

6. 12:15 am Carly Rolph Hobart and William Smith Colleges
Synthesis and Biological Evaluation of Simplified Analogs of Staurosporine
Oral Presentation Abstracts

Talk 1

“Green” Synthesis of Compounds with Biomedical Significance Facilitated by Water-Soluble Dendritic-Palladium Complexes

Eoghan L. Connors, Xin Liu and Ivan Gitsov*

Department of Chemistry and the Michael M. Szwarc Polymer Research Institute, SUNY College of Environmental Science and Forestry, Syracuse, NY

The Suzuki-Miyaura cross-coupling reaction (Suzuki reaction) is a highly efficient method of Carbon-Carbon bond formation, making it widely used in the synthesis of biaryl intermediates of pharmaceuticals. The coupling is conventionally performed at elevated temperatures and in organic solvents leading to adverse economic and environmental impacts. Previous studies in our group suggest that water soluble dendrimers, able to complex palladium, are viable Suzuki catalysts able to afford quantitative yields of the target compounds in water at close to ambient temperatures. They are, however, not ideal for catalyzing the reaction between hydrophobic reagents due to lack of contact with water-insoluble substrates. The goals of this study are to design and test water-soluble dendritic-palladium complexes containing a hydrophobic core, able to solubilize and selectively bind hydrophobic substances, in an attempt to improve the spatial arrangement of the catalyst and reagents in water. The structure of these novel “green” catalysts consists of calix[n]arene (n= 4,6,8) as the central core with water soluble poly(ester-ether) dendrons attached at the upper rim of the cycle (see figure below). This presentation will discuss our progress in the synthesis of these unique macromolecules by Williamson ether synthesis and Cu(I)-catalyzed alkyne-azide cycloaddition. Upon completion, this work aims to achieve unprecedented yields for the Suzuki reaction in water and produce the first Suzuki catalyst to mimic enzymatic character by selectively incorporating reagents.
Synthesis of Biaryl Precursors for the Bottom-Up Fabrication of Graphene Nanoribbons

Umar Asif\textsuperscript{1}, Brian Schultz\textsuperscript{2}, Sarbajit Banerjee\textsuperscript{2} and David G. Hilmey\textsuperscript{1}*  

\textsuperscript{1}Department of Chemistry, St. Bonaventure University, St. Bonaventure, NY  
\textsuperscript{2}Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Nanotechnology is becoming increasingly important in scientific applications, especially in electronics. Despite many advances, there is still need to increase the efficiency of production and determine nanochemical physical properties and how they affect function. A graphene nanoribbon (GNR) is an extremely thin, single layer of graphite less than 10 nm wide which can have properties ranging from metallic to semiconducting depending on the edge pattern. These differences define each nanoribbon.

In studying the bottom-up fabrication of graphene nanoribbons, dibrominated precursors have been prepared through electrophilic aromatic substitution and Suzuki coupling reactions. The synthetic strategies used are flexible to prepare a variety of monomers. These polyaromatics give rise to a variety of potential nanoribbons of different widths and edge properties. The dihalo monomers can be linked using surface-assisted coupling followed by subsequent cyclodehydrogenation to generate the desired nanoribbons.

In addition to the dihalo monomers which have been synthesized, current research involves the formation of bipyridyl compounds for similar purposes. Future directions will focus on continuing the synthesis of precursors, the fabrication of various GNRs, and the synthesis of zigzag GNR precursors.
Microwave-Assisted Synthesis of Thiazolidinedione Compound Library

Jason Biasini and Fehmi Damkaci*

Department of Chemistry, SUNY Oswego, Oswego, NY

Thiazolidinediones, also known as glitazones, are a class of medicinal compounds used in the treatment of diabetes mellitus type II, which are utilized in drugs such as Rosiglitazone and Pioglitazone. A library of thiazolidinedione derivatives has been synthesized using microwave irradiation over two steps, with an additional olefin reduction for select compounds yielding increased diversity. Numerous aromatic aldehydes and heterocyclic aromatic electrophiles have been tested and used in the production of the compound library. Several derivatives have been tested for medicinal activity against various biological targets by our collaborators in Japan, and more plan to be tested.
Calmodulin (CaM) is a highly conserved sensory protein whose unique structural geometry and range of flexibility have afforded a host of functions. Upon Ca$^{2+}$ binding to EF-hand loops, CaM drastically changes its conformation opening a hydrophobic cleft, where mutations can be introduced to confer catalytic activity onto this protein. We have previously demonstrated a single mutation in the active site of CaM can convert a non-enzymatic scaffold into a dynamic enzyme capable of catalyzing chemical transformations such as Kemp elimination and ester hydrolysis. Here we expand our minimalist approach to design an allosterically regulated retroaldolase. Specifically, we incorporated highly reactive lysine residues into CaM to facilitate carbon-carbon bond cleavage of β-hydroxy-ketones via a covalent Schiff base intermediate. Two mutants capable of catalyzing retroaldol reaction in methodol (CaM L105K and CaM F92K) were identified and characterized in detail. These promising results reveal that simple non-enzymatic proteins, such as calmodulin, can be engineered to assume novel catalytic functions.
[XeF$_5$]$^+$ and [Xe$_2$F$_{11}$]$^+$ Salts of the [Cr$^{IV}$F$_6$]$^{2-}$, [Cr$^V$OF$_5$]$^{2-}$, and [Cr$^V$$_2$O$_2$F$_8$]$^{2-}$ Anions

Daniel Stuart, James T. Goettel, Hélène P. A. Mercier and Gary J. Schrobilgen*

Department of Chemistry, McMaster University, Hamilton, ON

The known Cr(VI) oxide fluorides are represented by CrO$_2$F$_2$, CrOF$_4$, and [CrOF$_5$]$^-$. The latter anion has been characterized by means of vibrational spectroscopic studies of its [NO]$^+$ and Cs$^+$ salts. In the present work, the strong oxidative fluorinating agent, XeF$_6$, was reacted in varying molar ratios with CrOF$_4$, resulting in the formation of four new [XeF$_3$]$^+$ and [Xe$_2$F$_{11}$]$^+$ salts; [Xe$_2$F$_{11}$]$_2$[CrF$_6$], [XeF$_5$]$_2$[CrF$_6$]·2CrOF$_4$ (see Figure), [XeF$_5$][Cr$_2$O$_2$F$_8$], and [XeF$_5$][Xe$_2$F$_{11}$][CrOF$_5$]·2CrOF$_4$. The salts were characterized by single-crystal X-ray diffraction and provide the first crystal structures of the known [Cr$^{IV}$F$_6$]$^{2-}$ anion and the previously unknown [Cr$^V$OF$_5$]$^{2-}$ and [Cr$^V$_2$O$_2$F$_8$]$^{2-}$ anions. The formation of Cr(IV) and Cr(V) anions presumably result from reduction of Cr(VI) by elimination of O$_2$ and F$_2$, respectively.

Figure. The crystal structure of [XeF$_5$][CrF$_6$]·2CrOF$_4$; $P1$, $Z = 1$, $T = -173 \, ^\circ$C, $R_f = 0.023$. 
Synthesis and Biological Evaluation of Simplified Analogs of Staurosporine

Carly E. Rolph, Patricia Mowery and Erin T. Pelkey*

Departments of Biology and Chemistry, Hobart and William Smith Colleges, Geneva, NY 14456

Small molecular inhibitors of protein kinase C (PKC) represent promising therapeutic targets for a wide range of disorders, such as cancer, pain, heart disease and Alzheimer’s. Staurosporine, an indolocarbazole derivative, is a known PKC inhibitor. We are interested in the synthesis and biological evaluation of a new class of simplified staurosporine analogs, known as phenanthrene-fused 3-pyrrolin-2-ones (dibenzo[e,g]isoindol-1-ones). The synthesis of these new analogs was investigated using the oxidative cyclization of 3,4-diaryl-3-pyrrolin-2-ones. The launching of a new collaborative program for their biological evaluation will also be described.

Staurosporine

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\text{Me} \\
\text{Me} \\
\text{\hat{N}H} \\
\text{\textit{Simplified}} \\
\text{\textit{Me}} \\
\text{\textit{O}} \\
\text{\textit{Me}} \\
\text{\textit{Me}} \\
\text{\textit{O}} \\
\text{\textit{Me}} \\
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\]
**Student Poster Presentations**

**Time:** 1:30-3:30 PM  (Natural Sciences Complex, 2\textsuperscript{nd} Floor)

**Poster 1. Jose A. Barajas**, Jarrett A. Coppin, and Jason B. Benedict*  
*Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY*  
The Search for Sustainable Lighting: A Study of Co-Crystallized Organic Light Emitters

**Poster 2. Brandon M. Belz**, Scott J. Heller and Dominic L. Ventura*  
*Department of Math and Natural Sciences, D’Youville College, Buffalo, NY*  
Metallophthalocyanine–Catalyzed Wittig Olefination

**Poster 3. Christina Berti** and Kazushige Yokoyama*  
*Department of Chemistry, SUNY College at Geneseo, Geneseo, NY*  
Investigation of Peptide Self-Assembly at Interfacial Environment – Use of Thioflavin T Fluorescence

**Poster 4. Jonathan Binns**, Jamie Hitro, John Heck, Zachary Falls and Jeremy Steinbacher*  
*Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY*  
Toward a Multifunctional $^{19}$F MRI Contrast Agent Based on Mesoporous Silica Nanoparticles

**Poster 5. Erik Boldt** and Luis Sanchez*  
*Department of Biochemistry, Chemistry, and Physics, Niagara University, Niagara University, NY*  
Preparation of Complex Synthetic Building Blocks via Modification of L-Tryptophan

**Poster 6. Erick Braham** and Robyn E. Goacher*  
*Department of Biochemistry, Chemistry, and Physics, Niagara University, Niagara University, NY*  
Instrumental Analysis of Synergistic Enzyme Degradation of Lignocellulose

**Poster 7. Rachael M. Burke**, Kelly E. Henry and Robert P. Doyle*  
*Department of Chemistry, Syracuse University, Syracuse, NY*  
Delivering Appetite Suppression Peptides Through the Vitamin B12 Dietary Uptake Pathway
Poster 8. David R. Butzer, Dinesh G. Patel, Ian M. Walton, Jordan M. Cox, Cody J. Gleason and Jason B. Benedict*
Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY
Searching for Light Responsive Metal-Organic Frameworks via the Incorporation of Photochromic Linker Molecules

Poster 9. Matthew R. Crawley, Kate E. Pelcher, and Sarbajit Banerjee
Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY
“Smart” Window Coatings Integrating Vanadium Dioxide Nanowires within a Silica Matrix

Poster 10. Steven Dempsey and Luis Sanchez*
Department of Biochemistry, Chemistry, and Physics, Niagara University, Niagara University, NY
Studies Towards Novel Chemical Transformations of Vinylglycine

Poster 11. Jeffrey O. Ellison and Mark P. Heitz*
Department of Chemistry, The College at Brockport SUNY, Brockport, NY
Computational Study of Trihexyl(tetradecyl) Phosphonium Chloride Ionic Liquid Solvation

Poster 12. Gregory Faughnan, Renjith Maracheril and Kuppuswamy Arumugam*
Department of Chemistry, St. Bonaventure University, St. Bonaventure, NY
Electrochemical Control of Ring Size in the Catalysis of Cyclic Polyesters

Poster 13. Eric Helenbrook, Nick Turgeon and Kuppuswamy Arumugam*
Department of Chemistry, St. Bonaventure University, St. Bonaventure, NY
Exploration of N-Heterocyclic Carbene Annulated Oxalamide Derivatives and its Transition Metal Complexes

Poster 14. Guoqing Huang, Shuklendu D. Karyakarte and Sherry R. Chemler*
Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY
Synthesis of 1,4-Saturated Benzodiazepin-5-ones Via Copper Promoted Olefin Diamination

Poster 15. Stephanie M. Kong, Andrew M. Bodratti, Marina Tsianou and Paschalis Alexandridis*
Department of Chemical and Biological Engineering, University at Buffalo, SUNY, Buffalo, NY
Micellization of Alcohol Ethoxylate Surfactants
Poster 16. **Hyeokchan Kwon**, Brandon Bordeau, Ayal Adamit and Brian P. Callahan*

*Department of Chemistry, Binghamton University, SUNY, Binghamton, NY*

Expression and Refolding of the Autocatalytic HINT Domain from Human Sonic Hedgehog Protein

Poster 17. **Anthony V. Lake** and Matthew R. Gronquist*

*Department of Chemistry and Biochemistry, SUNY Fredonia, Fredonia, NY*

NMR Spectroscopy in the Analysis of Trapped Volatile Organic Compounds

Poster 18. **Maliek F. Likely**, Gregory Horrocks, and Sarbajit Banerjee*

*Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY*

Chemical Lithiation of V$_2$O$_5$ Nanowire Arrays Grown via Chemical Vapor Deposition

Poster 19. **Joseph C. Lumia** and Francis X. Webster*

*Department of Chemistry, SUNY College of Environmental Science and Forestry, Syracuse, NY*

Acetate and Formate Synthesis and the Practical Use of a Bromide Protecting Group

Poster 20. **Zachery P. McAtee** and Mark P. Heitz*

*Department of Chemistry, The College at Brockport SUNY, Brockport, NY*

Rheological Properties of Phosphonium Ionic Liquid/Methanol Solutions

Poster 21. **Robert Mroz** and Joseph LeFevre*

*Department of Chemistry, SUNY Oswego, Oswego, NY*

The Synthesis of Novel Betulin Derivatives.

Poster 22. **Christopher J. Reinhardt**, Xiang Zhai and John P. Richard*

*Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY*

Understanding the Role of Loop-Loop Interactions Through Mutagenesis Studies on Triosephosphate Isomerase

Poster 23. **Greg Sauer** and Mathew Vetticatt*

*Department of Chemistry, Binghamton University, SUNY, Binghamton, NY*

Transition State Analysis of Enantioselective Brønsted Base Catalysis by Chiral Cyclopropenimines
Poster 24. Dominic A. Sirianni, Naod Kebede* and Gerald J. Hoffman*
       Department of Chemistry, Edinboro University of Pennsylvania, Edinboro, PA

       Ab initio Study of 1,3,5-Trihydroxy-1,3,5-triazin-2,4,6[1H,3H,5H]-trione and its
       Decomposition Products

Poster 25. Michael F. Smith and Francis X. Webster*
       Department of Chemistry, SUNY College of Environmental Science and Forestry,
       Syracuse, NY

       Synthesis of 6Z,8E,10-Undecatrienyl Formate, the Major Sex Pheromone Analogue
       of the Carob Moth: Use of Bromine as a Formate Ester-Protecting Group

Poster 26. Angelina Sparano, Alex C. Levine* and Christopher T. Nomura
       Department of Chemistry, SUNY College of Environmental Science and Forestry,
       Syracuse, NY

       Characterization of Polyhydroxyalkanoate-based Electrospun Fibers

Poster 27. Bryna Torre,1 Samanthe Perera,2 Biplob Barmon,2 Joe Murphy,3 Haomin Song,3
       Qiaoqiang Gan,3 Alexander Cartwright,3 Athos Petrou2 and Hao Zeng3*
       1Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY
       2Department of Physics, University at Buffalo, SUNY, Buffalo, NY
       3Department of Electrical Engineering, University at Buffalo, SUNY, Buffalo, NY

       Synthesis of Hybrid Perovskite Material for Optoelectronics Applications

Poster 28. Jenny Tse, Sarina Blum, Yuanyuan Wang1*, Thomas Zengeya2, Karl Wilson1,
       Anna Tan-Wilson1 and Eriks Rozners2
       1Department of Biology, Binghamton University, Binghamton, NY
       2Department of Chemistry, Binghamton University, Binghamton, NY

       Capture of Proteases Using Peptide Nucleic Acid-Based Probes

Poster 29. Lauren E. VanGelder, Christopher C. Mielleville, Kate E. Pelcher, Sarbajit
       Banerjee and David F. Watson*
       Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

       Functionalization of Single-crystalline β-Pb_xV_2O_5 Nanowires with Light-harvesting
       Cys-CdSe Semiconductor Quantum Dots

Poster 30. Cody C. Webb Jr., Alan Goos, Anna O’Brien and Karin Ruhlandt-Senge*
       Department of Chemistry, Syracuse University, Syracuse, NY

       Structural and Volatility Investigations of Fluorinated Bismuth Metallorganics
The Search for Sustainable Lighting: A Study of Co-Crystallized Organic Light Emitters

Jose A. Barajas, Jarrett A. Coppin, and Jason B. Benedict*

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Phosphorescent organic light emitting diodes (POLEDs) have the potential to serve as more efficient light emitters than conventional light emitting diodes (LEDs). Currently the most efficient POLEDs are organometallic complexes containing precious metals such as titanium or iridium. In order to create more efficient and sustainable POLEDs, crystallographic research has been conducted on purely organic mixed crystals. This research focuses on known phosphors such as benzophenone (BP) and various BP derivatives. Samples were co-crystallized and analyzed using x-ray diffraction and prepared for time-resolved spectroscopy to study the photophysical characteristics.
Metallophthalocyanine–Catalyzed Wittig Olefination

Brandon M. Belz, Scott J. Heller and Dominic L. Ventura*

Department of Math and Natural Sciences, D’Youville College, Buffalo, NY

The Wittig reaction to synthesize olefins is a very attractive method in organic synthesis. Recently, this methodology has been achieved utilizing simple metal catalysts and diazo compounds in addition to a phosphine and an aldehyde. We report, for the first time, this chemistry being catalyzed by metallophthalocyanines. The following work investigates the use of a variety of these organometallic complexes to catalyze Wittig-like reactions from ethyldiazoacetate. We also examine the influence of substitution on the aromatic ring of the aldehyde as well as various phosphines, arsines and antimony complexes. We have been able to exclusively synthesize the trans-olefins in excellent yields in short periods of time (1 hour).

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\begin{align*}
    \text{Ph} & \rightarrow \text{H}_{2}\text{N} & \rightarrow \text{H}_{2}\text{COOEt} & \rightarrow \text{Ph} = \text{H, Me, OMe, Ph, Cl, F, Br, CF}_{3}, \text{NO}_{2} \\
    \text{MPc} & = & \text{M} = \text{Ag, Co, Cu, Fe, Ni, Zn} \\
\end{align*}
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Poster 3

Investigation of Peptide Self-Assembly at Interfacial Environment – Use of Thioflavin T Fluorescence

Christina Berti and Kazushige Yokoyama*

Department of Chemistry, SUNY College at Geneseo, Geneseo, NY

Alzheimer’s disease in the most common form of dementia witnessed in elderly adults, as it affects over 30 million people worldwide. The essential focus of this research is to study the first two proposed steps of fibrillogenesis, the process responsible for aggregation of amyloid β fibrils which constitute characteristic extracellular senile plaques. Analysis is executed by the utilization of enhanced Thioflavin T (ThT) fluorescence upon binding amyloid β fibrils. Under the assumption of previously reported means of ThT binding to amyloid β fibrils, we investigate the spectra in an attempt to assign potential conformations of amyloid fibrils to the observed fluorescence peaks. So far, our results provide evidence that enhanced ThT fluorescence in the presence of amyloid β 1 – 40 is most prominently demonstrated in basic solution conditions (~pH 9 – pH 10). In continuation of this study, we plan to test for any reversibility in observed fluorescence with respect to pH fluctuations; we also wish to study the effect of other changes in medium environment. All performed fluorescence tests are carried out using chicken ovalbumin.
Toward a Multifunctional $^{19}$F MRI Contrast Agent Based on Mesoporous Silica Nanoparticles

Jonathan Binns, Jamie Hitro, John Heck, Zachary Falls and Jeremy Steinbacher*

Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY

Novel drug-delivery agents are needed to overcome the limitations of systemic toxicity of traditional chemotherapeutics, and an even more powerful paradigm combines delivery and imaging into one agent. One potential platform for such an agent is nano- or microparticles consisting of mesoporous silica, a well-characterized material with minimal toxicity and with great flexibility for chemical functionalization. Much progress has been made using porous silica particles as multifunctional drug-delivery agents, enabling combined delivery and imaging by incorporating contrast agents for optical detection, PET, and proton MRI. One imaging modality not yet combined with porous particles is $^{19}$F MRI.

Here, we present efforts to prepare a multifunctional silica nanoparticle that incorporates fluorine atoms for detection by $^{19}$F MRI. We have synthesized several alkoxysilanes that contain multiple, chemically-equivalent fluorine atoms in the form of trifluoromethyl groups. We have subsequently immobilized these silanes to the pore surfaces of mesoporous silica nanoparticles (with the MCM-41 pore structure) that were PEGylated on their exterior surfaces to promote biocompatibility and water-dispersibility. Lastly, we used $^{19}$F NMR spectroscopy to detect these immobilized fluorine atoms and measure their magnetic relaxation properties, demonstrating proof-of-principle that $^{19}$F MRI could be used to detect and image these materials. Relaxation rates and signal-to-noise ratios were sufficient to acquire spectra in short amounts of time. In related work, we are preparing stimuli-responsive alkoxysilanes, which could be used to effect a “switch-on” response in $^{19}$F MRI, that respond to changes in pH or reducing conditions.
Preparation of Complex Synthetic Building Blocks via Modification of L-Tryptophan

Erik Boldt and Luis Sanchez*

Department of Biochemistry, Chemistry, and Physics, Niagara University
Niagara University, NY

Members of the moroidin and celogentin families of natural products, among others, contain structural moieties based on substituted/oxidized L-Tryptophan units. Studies have found that many of these compounds have properties of biomedical relevance. In order to prepare complex structures in a cost-effective manner, it would be ideal to use natural amino acids or other widely available, low-cost feedstocks as starting points. Surprisingly, elaborate molecules are most commonly prepared from other materials, usually petroleum-based, to showcase particular methodologies. This study aims to identify efficient yet simple methods of producing tailored derivatives of tryptophan as building blocks for complex molecule synthesis.
Poster 6

Instrumental Analysis of Synergistic Enzyme Degradation of Lignocellulose

Erick J. Braham and Robyn E. Goacher*

Department of Biochemistry, Chemistry, and Physics, Niagara University, Niagara University, NY

Green energy is an exciting field of study in our modern world. One renewable resource is plant matter and this has the potential as a fuel for the future. To harness this energy we must convert plant matter into useful products. One possible way to achieve this is with the help of enzymes. This study looks into how two of those enzymes (laccase/xylanase) work together synergistically to break down plants to create useful products. This poster discusses our approach to finding the right mixture of enzymes, analytical approaches, and preliminary results.
Obesity has emerged as a significant problem in today’s society. Peptide YY (PYY) has been shown to have clinical relevance in appetite control with studies showing that a truncated form of PYY, PYY3-36, inhibits food intake in rodents, primates, and humans. The anorectic effect PYY3-36 causes is due to agonism of the Y2 receptor in the hypothalamus. The focus of this research is to develop an oral delivery route for exogenous PYY3-36 that elicits in vivo agonism through utilization of the B12 dietary uptake pathway. The hypothesis of the research is that the B12 pathway can be utilized to protect and actively transport select peptides through the gastro-intestinal tract, delivering them to blood. Herein we will discuss the synthesis, characterization, and in vitro pharmacodynamics of two B12-PYY3-36 conjugates with tailored functionality at the Y2 receptor.
Poster 8

Searching for Light Responsive Metal-Organic Frameworks via the Incorporation of Photochromic Linker Molecules

David R. Butzer, Dinesh G. Patel, Ian M. Walton, Jordan M. Cox, Cody J. Gleason and Jason B. Benedict*

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Photochromic molecules have the potential to transform traditionally passive materials into active materials which change their chemical or electronic properties in response to light stimulus. Photochromic molecules can be combined with metal-organic frameworks to create advanced materials for chemical separation, sensing, and photo-mechanical actuation. To further investigate, various photochromic linker molecules were synthesized to then be incorporated into metal organic frameworks. The photochemical reactions in these materials, both desired and undesired, were precisely monitored through spectroscopic and X-ray diffraction methods.
Increasing the efficiency of heating and cooling of residential and commercial buildings is an urgent imperative given that 40% of all energy consumption in the United States occurs within buildings. Thermally responsive “smart” window coatings offer a convenient and facile route to solving this problem and reducing energy costs. We have attempted to design spectrally selective and thermally responsive coatings based on nanowires of vanadium dioxide (VO$_2$). VO$_2$ exhibits an unusual metal—insulator transition accompanied by orders of magnitude change in optical transparency. In previous work, the transition temperature of 67°C characteristic for bulk VO$_2$ has been tuned to lower (more relevant for fenestration) temperatures by using a variety of dopants along with scaling into the nanometer-sized regime. In order to form a durable coating for consumer applications, a unique approach is presented for chemically integrating the VO$_2$ nanowires onto glass substrates. A modified Stöber method is utilized to affix a silica shell to the surface of VO$_2$ nanowires. The reaction solution is then directly spray coated onto a cleaned glass substrate, resulting in a chemically bonded VO$_2$/SiO$_2$ coating. Variations of the parameters of the VO$_2$ suspension yield a wide range of coatings and allows for development of structure—function correlations. Scanning electron microscopy enables examination of the surface morphology of the coatings and infrared spectroscopy is employed at a range of temperatures to examine how the optical transmittance varies as a function of temperature. Infrared spectroscopy results indicate a decrease in transmittance by approximately 40% at high temperatures.
Poster 10

Studies Towards Novel Chemical Transformations of Vinylglycine

Steven Dempsey and Luis Sanchez*

Department of Biochemistry, Chemistry, and Physics, Niagara University
Niagara University, NY

Vinylglycine is a unique amino acid that has been the target of a number of synthetic studies in the past. Elaborate forms of its structure, which are still difficult to access, are observed in many natural products of biological significance. The present project aims at identifying a convenient scalable synthesis of vinylglycine and exploring chemical transformations of its molecular structure. We anticipate incorporating vinylglycine in the preparation of much larger complex molecules taking advantage of its alkene moiety.
Computational Study of Trihexyl(tetradecyl) Phosphonium Chloride Ionic Liquid Solvation

Jeffrey O. Ellison and Mark P. Heitz*

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Ionic liquids are of particular interest because they offer an “environmentally friendly” alternative to volatile organic hydrocarbon (VOC) solvents. One principle of green chemistry promotes the use of innocuous solvents in chemical processing. The goal of our research is to determine the solvation energetics of ionic liquids when dissolved in conventional solvents such as methanol (MeOH) and water. The ionic liquids used in this work are based on the trihexy(tetradecyl)phosphonium cation (P\textsubscript{14,6,6,6}\textsuperscript{+}, PIL). To date we have studied the solvation of PIL with chloride and bromide anions. The PIL systems were modeled computationally using Spartan14\textsuperscript{®} software using different levels of theory and basis sets, including AM1, PM3, and PM6 semiempirical methods and Hartree Fock \textit{ab initio} methods with 3-21G and 6-31G basis sets. Solvation was computed using continuum dielectric solvents with SM5.4 and SM8 solvent models. The optimum cation/anion separation (energy minimum) was determined by calculating the interaction energy in both vacuum and solvent. In vacuum PILCl has an optimum separation of 0.337 nm compared to PILBr which has an optimum separation of 0.405 nm, consistent with the trend in anion ionic radius. Solvation energies of solvated ion pairs and solvent separated ions were computed for all solvents studied and are discussed in this work.
Poster 12

**Electrochemical Control of Ring Size in the Catalysis of Cyclic Polyesters**

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*N*-Heterocyclic carbene (NHC) facilitated zwitterionic ring-opening polymerization of lactones has proved a useful technique in the synthesis of cyclic polyesters. Previous control of ring-size has been dependent on monomer concentration and no methods for recycling NHC catalysts have been reported, however, use of metal bis(dithiolene) complexes show promise. Different metal bis(dithiolene) complexes and NHC combinations are being investigated for catalyst optimization.
Poster 13

Exploration of N-Heterocyclic Carbene Annulated Oxalamide Derivatives and its Transition Metal Complexes

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By further investigating the electronic nature of N-heterocyclic carbenes (NHCs), which act as great donor ligands, we attempted to modify the oxalamide backbone to complex with various transition metal complexes in hopes to find better fluorescent materials. After successful synthesis and characterization, these materials will be subjected to extensive absorption and fluorescence measurements.
Benzodiazepines and benzodiazepinones are known for their psychoactive properties in the pharmaceutical field; for example, they can be used to treat many diseases and symptoms that have correlations with the central nervous system. A novel synthesis of these benzodiazepinone structures is disclosed herein. The method involves copper ethylhexanoate promoted alkene diamination/cyclization in presence of an external nitrogen nucleophile source to yield these benzodiazepinones in good yields.

Scheme:
Micellization of Alcohol Ethoxylate Surfactants

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We consider non-ionic surfactants in terms of their ability to stabilize oil-in-water emulsions or dislodge oil adsorbed on surfaces, on their own, or in a formulation containing other surfactants (ionic and/or non-ionic) or nanoparticles. Fundamental information about the micellization of surfactants in aqueous solution can be used to assess the compatibility and potential synergism with other surfactants, and the surfactant affinity to oil. We examine here a homologous series of surfactants consisting of a single-branch C10-alcohol with varying degrees of ethoxylation, and report results on the onset of micellization (cmc), micellization thermodynamics, and local environment in the micelles formed in aqueous solutions in the presence of cosolvents and electrolytes.
Expression and Refolding of the Autocatalytic HINT Domain from Human Sonic Hedgehog Protein

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The Sonic Hedgehog (SHh) protein is one of three mammalian signaling proteins in the hedgehog family. Its physiological roles include regulation of human embryo development while also having pathogenic activity in cancers of the prostate, breast, and pancreas. Here we report conditions to express, purify, and refold the autocatalytic domain of SHh, called HINT, for future structure/function studies. We demonstrate that the refolded HINT domain undergoes a self-cleavage reaction which is known to be a critical step in SHh biosynthesis. Ongoing work aims to prepare refolded HINT in amounts suitable for structural studies using NMR.
NMR Spectroscopy in the Analysis of Trapped Volatile Organic Compounds

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Methods for the collection and analysis of volatile, small-molecule chemical signals have applications in areas such as food science, air-quality analysis, and chemical ecology. A commonly employed strategy involves trapping gas phase small-molecules emitted from a sample onto a solid-phase adsorbent trap, followed by subsequent desorption and analysis by gas chromatography. We are investigating the feasibility of nuclear magnetic resonance (NMR) as a complimentary or alternate means of analysis for collected samples. By directly desorbing volatiles from adsorbent traps using deuterated solvents, NMR spectra may be acquired prior to further analysis by other methods, providing an additional level of structural information for mixtures of trapped volatiles. Using one and two-dimensional NMR techniques, volatiles from lemon balm, basil, and sage were analyzed.
Chemical Lithiation of V$_2$O$_5$ Nanowire Arrays Grown via Chemical Vapor Deposition

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Lithium-ion batteries are plagued by low energy densities and poor cyclability with the latter arising from the gradual degradation of electrodes due to the stresses generated from volume expansions and contractions with lithium insertion/removal. Scaling materials to nanometer-sized dimensions represents an attractive solution to these problems. Vanadium(V) oxide (V$_2$O$_5$) has been the subject of much investigation for use as a cathode material in lithium-ion batteries. The facile accessibility of the V$^{5+}$/V$^{4+}$ redox couple and the layered structure of V$_2$O$_5$ allows for the insertion and extraction of lithium ions from interstitial sites. V$_2$O$_5$ has a high energy density owing to the large available space for the intercalation of lithium ions and the ability to access the V$^{4+}$/V$^{3+}$ redox couple in addition to the V$^{5+}$/V$^{4+}$ redox couple.

Arrays of oriented quasi-1D nanostructures are an attractive improvement upon traditional bulk materials, and continuous films given the greater surface area for interfacing with an electrolyte and their potential to individually maintain electrical contact to a current collector. Chemical vapor deposition allows for the synthesis of oriented arrays of nanostructures that are densely packed and anchored to a conducting substrate. The nanoscale size of these arrays shortens the average path length for Li insertion allowing for faster cycling; whereas, the increased freedom to accommodate strain allows nanostructures to repeatedly change volume upon cycling without degradation. This study shows the synthesis of such arrays, and their ability to reversibly accommodate the insertion and removal of lithium ions. Specifically, we have used Raman spectroscopy and X-ray diffraction to track changes in structure of the V$_2$O$_5$ nanowires with increasing extents of lithiation.
Poster 19

Acetate and Formate Synthesis and the Practical Use of a Bromide Protecting Group

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Alkyl bromides are often considered very reactive and would not be considered as a protecting group. There is also a dearth of useful methods for converting bromides to alcohols under mild conditions. Alkyl bromides are however, quite stable to a wide range of conditions and a carefully planned synthetic scheme will allow for its use in many reaction pathways. The key to using bromides in this regard will be use of carboxylic acid salts to convert the alkyl bromide to an ester (acetate or formate).

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\text{7Z,9E,11-Dodecatrienyl Formate}
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In a reaction scheme for a female carob moth sex pheromone a bromide will be used as a protecting group at one end of the molecule (left side). The bromide will be considered as a protecting group for alcohols and their derivatives. A mono-substituted bromoalcohol was formed. A 2.5 meq of sodium acetate or formate to bromoalcohol in DMSO and water at 100°C yielded the monoacetate or monofomate. Results were confirmed by NMR and GC. Both bromooctane and chloropentane successfully formed the acetate or formate via these methods. Preliminary results for a secondary chloride show no reaction occurred. Monosubstituted vs. disubstituted products are time- and temperature-dependent. Using water as a starting material produced alcohol. Removing water eliminated alcohol production. To determine if a bromide can be considered a protecting group, the following reactions will be tested: Jones and Corey oxidations, LAH reduction, alkylation by a Grignard reagent, and hydrogenation by P₂/Nickel. Early results show bromides are robust under both oxidation and Grignard alkylation.
Rheological Properties of Phosphonium Ionic Liquid/Methanol Solutions

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Ionic liquids are considered to be environmentally friendly solvents and are therefore used as alternatives to harsh volatile organic hydrocarbon (VOC) solvents. The goal of our research is to determine how the mass transport variables, specifically density and viscosity, of the ionic liquid trihexy(tetradecyl)phosphonium chloride (PILCl) change as a function of temperature and mol fraction ionic liquid. The choice of methanol as the cosolvent is driven by previous experiments in our lab, which have shown that PILCl is most miscible with methanol in contrast to longer chain alcohols or other traditional organic solvents such as dichloromethane, THF, hexane, etc. Specifically we have measured density and viscosity of methanol solutions across the entire range of mol fraction (x_{PILCl} = 0 - 1) and over a temperature range of 17 to 50°C. The viscosity data generally follows Stokes-Einstein behavior and shows a linear proportionality to mol fraction. Excess molar volumes are also computed from the density data and are overall negative suggesting that on mixing the solution volume collapses due to intermolecular hydrogen bonding.
The Synthesis of Novel Betulin Derivatives.

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Betulin, a naturally occurring compound abundant in birch bark, has shown cytotoxicity towards a variety of cancer cell lines, strong anti-inflammatory activity and substantial anti-HIV activity, specifically in the diester derivative form. The TI and EC$_{50}$ values of betulin diester derivatives are comparable to the TI and EC$_{50}$ values of Zidovudine (AZT), a powerful FDA approved anti-HIV medication. The effectiveness of an anti-viral and anti-cancer compound is often limited by poor water solubility, directly affecting the potency of the compound. The versatile structure of betulin makes it an ideal candidate for modifications using conventional synthetic organic approaches. By altering the chemical structure of betulin slightly through the addition of appropriate amino acid groups, the solubility of the compound can be increased. The overall goal of the work is to synthesize ten to fifteen new betulin diester derivatives while striving to optimize the reaction conditions. Currently five amino acids have been successfully coupled through traditional reflux. The betulin-amino acid coupling reaction has already been significantly improved as well. The total reaction time was reduced from 48 hours to 4 hours through the use of practical Microwave Assisted Organic Synthesis (MAOS). The current status of this work will be presented.
Understanding the Role of Loop-Loop Interactions Through Mutagenesis Studies on Triosephosphate Isomerase

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Triosephosphate isomerase (TIM) utilizes desolvation of the active site and electrostatic interactions to efficiently catalyze the isomerization reactions between D-glyceraldehyde-3-phosphate (D-GAP) and dihydroxyacetone phosphate (DHAP). Upon substrate binding, TIM’s loop 6 closes and situates the catalytic base towards the substrate for proton abstraction. Loop 6 is stabilized in the closed conformation through interactions with loop 7. Inhibition studies with 3-phosphoglycolic acid (PGA), a transition state analog, were conducted on Y208 mutants to elucidate its role in stabilizing the close, active conformation. The results suggest that the tyrosine residue is involved in the facilitation of loop-6/7 hydrogen bonding. The Y208T mutation had little effect on the pKₐ of the active catalytic base, E165. Y208A and Y208F mutants perturbed the pKₐ of E165, resulting in values of 9.0 and 7.5 respectively. This variation indicates that more than one hydrogen bond is involved.
Poster 23

Transition State Analysis of Enantioselective Brønsted Base Catalysis by Chiral Cyclopropenimines

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Recently, the Lambert group at Columbia University reported on the use of a chiral 2,3-bis(dicyclohexylamino) cyclopropenimine as a catalyst for the Michael addition of glycinate imines to benzyl acrylate in high yield and enantioselectivity. In the interest of new reaction development and catalyst design, we undertook the task of a mechanistic study. Measurement of $^{13}$C kinetic isotope effects (KIEs) revealed that the reaction proceeds via rate-limiting carbon-carbon bond formation. The key catalyst-substrate interactions and the origin of enantioselectivity are identified based on DFT calculations using various calculational methods. The transition state leading to the observed enantiomer of product is found to accurately predict the experimental KIEs. The transition state model is expected to guide future reaction development with this unique catalyst.

Coupling of glycine imine 2 with acrylate 3 in the presence of catalyst 1, our system of interest

Kinetic Isotope Effects and Preliminary computational results
Ab initio Study of 1,3,5-Trihydroxy-1,3,5-triazin-2,4,6[1H,3H,5H]-trione and its Decomposition Products

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1,3,5-trihydroxy-1,3,5-triazin-2,4,6[1H,3H,5H]-trione, also referred to as trihydroxy isocyanuric acid (THICA), is a stable trimer of the elusive N-hydroxyisocyanate, HONCO. The dissociation of THICA is believed to proceed by producing three HONCO intermediates, which then further dissociate to yield HNO and CO. There has been no definitive experimental observation of HONCO as a stable molecule. We present the results of ab initio calculations on THICA and HONCO, as well as the final products, CO and HNO. Calculations are performed at the level of Hartree-Fock self-consistent field theory (HF-SCF), Møller-Plesset second-order perturbation theory (MP2), coupled-cluster theory including singly and doubly excited configurations (CCSD), as well as inclusion of noniterative triple excitations (CCSD(T)); a variety of basis sets were used. Structural data, vibrational frequencies, and atomic charges are presented; it is hoped that calculated vibrational frequencies for HONCO will aid in its experimental identification. We have identified a transition state in HONCO, indicating a pathway for dissociation in the ground state. Ultimately, excited state potential surfaces for both HONCO and THICA will be explored to investigate dissociation pathways in each of these species.
Poster 25

Synthesis of 6Z,8E,10-Undecatrienyl Formate, the Major Sex Pheromone Analogue of the Carob Moth: Use of Bromine as a Formate Ester-Protecting Group

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The carob moth, *Ectomyelois ceratoniae*, is a pest of nut and fruit crops. Use of synthetic pheromone traps to monitor and detect populations can help reduce and even eliminate losses due to infestations. The analogue compound 6Z,8E,10-undecatrienyl formate 1 is related to a known mimic of the major sex pheromone of the carob moth. We report the nine step synthesis of this important pheromone analogue using bromine as a successful formate ester-protecting group. The primary alkyl bromide proved to be “inert” through several different types of reactions. The key step is the conversion of an allene to a (Z,E) conjugated diene using basic Al₂O₃.

![Chemical Structure](image_url)
Characterization of Polyhydroxyalkanoate-based Electrospun Fibers

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Polyhydroxyalkanoates (PHAs) are biopolymers that can be made using recombinant Escherichia coli (E. coli) and have potential to be used in a broad range of applications including drug delivery, carbon storage, and even as precursors for biofuels. PHAs can be electrospun into fibers that can be very useful for the environment or healthcare industry. In this experiment we studied the production and characterization of PHA electrospun fibers. These fibers were characterized using Scanning Electron Microscopy (SEM) to observe fiber morphology. The PHA fibers were doped with carbon nanotubes (CNTs) that were sonicated into the electrospinning solution to make it easier to embed in the fibers. The purpose of the carbon nanotubes is to make the films stronger. It is predicted that well-made PHA-based fibers will have a very small diameter (0.5-5 microns), no beading, and evenly dispersed carbon nanotubes. A solution of 1:4 dimethylformamide:chloroform was found to be the optimal solvent for the electrospinning process. This combination yielded the most uniform fibers with little to no beading, which were about 3 µm in diameter. Future work will include tensile strength tests that test the amount of tension that can be placed on the film.
Poster 27

Synthesis of Hybrid Perovskite Material for Optoelectronics Applications

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Hybrid organic/inorganic perovskite (i.e. CH$_3$NH$_3$PbI$_3$) is a class of emerging semiconducting material with large absorption coefficient and long carrier diffusion length. They have demonstrated tremendous potential for photovoltaics, yielding power conversion efficiency above 15% in a short time. Low threshold amplified spontaneous emission was also observed in solution processed mixed halide perovskites, demonstrating their potential for lasing. In this work, we report the synthesis of perovskite films using vapor assisted method, in which CH$_3$NH$_3$I was evaporated and reacted with solution deposited PbI$_2$, based on an earlier report. X-ray diffraction confirms the structure of the as-deposited films. UV-vis absorption and photoluminescence (PL) shows the band gap for CH$_3$NH$_3$PbI$_3$ to be ~1.63 eV. The films have unconventional temperature dependent PL energy: it first increases from 1.60 eV at 300 K to a peak value of 1.70 eV at 150 K, and decreases with further lowering of temperature. This is attributed to a transition from excitonic emission at low temperatures to band edge emission at high temperatures. The exciton binding energy is estimated to be of the order of a few ten meV. Mn$^{2+}$ ions were substitutionally doped to induce carrier spin polarization. A second temperature independent peak at 2.1 eV was observed, possibly due to the ligand field transition of Mn$^{2+}$ coordinated with six I$^-$ ions. The results on time-resolved PL will also be discussed.
Capture of Proteases Using Peptide Nucleic Acid-Based Probes

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Commercially available probes that capture active proteases in biological tissue, also known as activity based protein profiling (ABPP), make use of reagents that recognize the active site and also provide a quick way for protein isolation. The latter systems are imperfect because they require the dissociation of the biotin from the streptavidin coated beads. Harsh eluting conditions required result in leaching streptavidin and other contaminating materials that hinder the identification of the tagged proteins. Peptide nucleic acid (PNA)-based probes were designed to take advantage of the high affinity between biotin and streptavidin, while eliminating the need to dissociate the complex. We synthesized a probe consisting of two complementary 8-bp PNA strands. PNA-I was conjugated with iodoacetic acid for capturing proteases that depend on a nucleophilic sulfhydryl group for activity, at their optimal pH. PNA-B was covalently linked with biotin for magnetic bead separation of the proteases from protein extracts. The proteases are released simply by application of heat (60°C) for 5 mins. This was tested successfully by capturing pure papain, a commercially available purified cysteine protease at pH 6.2.
Functionalization of Single-crystalline $\beta$-Pb$_x$V$_2$O$_5$ Nanowires with Light-harvesting Cys-CdSe Semiconductor Quantum Dots

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Lead vanadium oxide ($\beta$-Pb$_x$V$_2$O$_5$) is a semiconductor which has potential as a photocathode in photoelectrochemical cells due to its wide-band gap and mid-gap electronic states. This poster will report our results involving the functionalization of $\beta$-Pb$_x$V$_2$O$_5$ nanowires with light-harvesting CdSe semiconductor quantum dots (QDs), toward the goal of promoting excited-state interfacial charge separation. Tunability in both the mid-gap states of the nanowires and the band gap of QDs allows for band alignment at the nanowire-QD interface, which results in a thermodynamic driving force for hole transfer from the valence band of the QD into the mid-gap states of the $\beta$-Pb$_x$V$_2$O$_5$ nanowires. The approach utilized for quantum functionalization on nanowires is linker-assisted CdSe attachment via the bifunctional linker cysteinate$^{2-}$ (Cys). Preliminary results indicate promising evidence of linker attachment to $\beta$-Pb$_x$V$_2$O$_5$ nanowires.
Poster 30

Structural and Volatility Investigations of Fluorinated Bismuth Metallorganics

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Mixed metal electronic thin films such as Bi$_2$Sr$_2$CaCu$_2$O$_x$ are prepared by metal-organic chemical vapor deposition (MOCVD). Preferred precursors for MOCVD contain multiple metal species and are highly volatile, while maintaining thermal stability during sublimation. Common bismuth precursors include Bi(C$_6$H$_5$)$_3$, however single source alkaline earth bismuthate heterobimetallic precursors have yet to be developed. Our group has previously developed a series of alkaline earth metal MOCVD precursors which used the perfluoro-tert-butoxide (PFTB) ligand, affording unprecedented volatility. Based on these results, we report here a new series of bismuth precursors using PFTB. These complexes were synthesized by a solvent-free benzene elimination reaction using BiPh$_3$ and crystals were extracted using tetrahydrofuran (THF), pyridine, diethyl ether (Et$_2$O), 1,2-dimethoxyethane (DME), N,N,N’,N’-tetramethyldiethylenediamine (TMEDA), and diethylene glycol dimethyl ether (diglyme). Structural studies by single-crystal X-ray crystallography have shown probable bridged dimers for TMEDA-, DME-, and Et$_2$O-adducts, and facial and meridinal octahedral THF- and pyridine-adducted complexes, respectively. The volatility of these complexes was studied by thermalgravimetric analysis. Future research will focus on homoleptic heterobimetallic alkaline earth bismuthates using the PFTB ligand.