Thank you to the following groups for their support of this symposium:

University of Notre Dame: Biology REU Program, Center for Research Computing, Center for Sustainable Energy at Notre Dame, Center for Undergraduate Scholarly Engagement, College of Science, Graduate School, Harper Cancer Research Institute, and NDnano and Physics REU Program

University of Michigan: Chemistry REU program
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Oral Presentations Schedule  
Biology, Chemistry, Engineering, and Humanities  
Jordan Room 105

Session I  
11:00 am - 12:00 noon

Moderator: Dominic Chaloner

11:00 Karolina Gogola - ARID3B regulates stem cell adhesion through CD133  
11:15 Alexandra Santiago - A comparative look on the conflicts in the Sahel Region  
11:30 Nirbhay Jain - A Simple Method of Minimizing Ionic Strength to Reduce Chemical Shift Variation in NMR-based Metabolomics of Urine Specimen  
11:45 Stephen Ennis - Dynamic Provisioning of Custom Clusters Through HTCondor and Openstack

Session II  
2:00 pm – 4:00 pm

Moderator: Elena Brindley

2:00 Luqun Shen - Developing an Effective Immunotoxin that Targets Cells Overexpressing ErbB2  
2:15 Abigail Shepard - Blinded by the Light: A Vitamin B₁₂ Kinetics and Quantum Yield Study  
2:30 Francis Rogg - Providing Better Tools for Responsible Design  
2:45 Santiago Martinez - Synthesis of Silver Nanoparticles in Microdroplets Using a Plasma Jet  
3:00 Esseabai Etim - Building a Database for Automated Paper Analytical Devices Analysis  
3:15 Emmanuel Sosa - Italianizing History  
3:30 Ning Zhou - Effect of Antagonists on Heteromerization of NMDA Receptor Ligand Binding Domains
Physics

Jordan Room 322

Session I
9:00 am - 10:30 am

Moderator: Umesh Garg

9:00  Steven Hyatt - Modeling the Accretion and Feedback Rates of Galaxies Similar to the Milky Way
9:13  Marina Paggen - Filaments: Understanding the Math that Defines them
9:26  Adrian Rivera-Torres - Fluid Dynamics - From Helping Messi Goal to Modeling the Evolution of a Galaxy
9:52  Mitch McNanna - Natural orbitals for a two-particle system in one dimension as a testbed for use in the nuclear many-body problem
10:05 Jason Saroni - Analysis of schematic one-level and two-level nuclear shell models
10:18 James St Germaine-Fuller - Coupling Algorithm for Sp(3,R) Irreducible Representations

Session II
10:45 am - 12:15

Moderator: Umesh Garg

10:45  Patrick Fasano - Modernizing Plunger Control with Low-cost Digital Electronics
10:58  Timothy Khouw - Nuclear Data Made Easy with the Notre Dame Nuclear Database
11:11  Marcus Lowe - Measurements of Internal Conversion Electron Emission Cross-Sections for 154, 156, 157Gd
11:24  Luis Abrego Rangel - Characterization of thin foils as target materials for nuclear reactions
11:37  Patricia Huestis - Modal noise mitigation in optical fibers with small circular diameters
11:50  Chuanhong Liu - Search for Gamma-Ray Sources from a Measurement of the Muon Angular Distribution with High Statistics
12:03  Zeyu Hao - Gamma-ray Burst Analysis in Project GRAND and Flares Seeking in UW Crb
Physics  
Jordan Room 322

Session III  
2:00 pm – 3:30 pm

Moderator: Umesh Garg

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<tr>
<td>2:00</td>
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<td>2:13</td>
<td>Devon Courtwright - Investigating the Magnetic Properties of Metal/Semiconductor Hybrid Samples</td>
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<td>2:26</td>
<td>Allan Leishman - Accelerating the Analysis of SANS of Superconducting Vortex Lattices</td>
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<td>2:39</td>
<td>Kevin Howard - Study of the pure double folding optical model for 100 MeV/u deuteron scattering</td>
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<td>Emily Morgan - Analyzing Deuteron Scattering at 100 MeV/u Through Optical Model Parameters</td>
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<td>3:05</td>
<td>Benjamin Guerin and Lindsey Riordan - Graphitization Line for AMS Measurement of Carbon-14</td>
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<td>Daniel Votaw - Finding the optimal parameters for use of a position-sensitive ionization chamber</td>
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Session IV  
3:58 pm - 5:15 pm

Moderator: Umesh Garg

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<td>3:58</td>
<td>Guillermo Bustos-Ramirez - How to produce slow radioactive ion beams</td>
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<tr>
<td>3:45</td>
<td>Catherine Nicoloff - Simulating a Multi-Reflection Time-of-Flight Mass Spectrograph for the Purification of Radioactive Isobars</td>
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<td>4:11</td>
<td>Michelle Gervais - Alignment Sensitivity Study of the St. ANA Beam Line</td>
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<td>4:24</td>
<td>Andre Wilson - High Purity Germanium Detectors and Angular Distribution of 27Al(p,γ)28Si</td>
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<td>4:37</td>
<td>Yi Jia - Beamline optimization for Long Baseline Neutrino Experiment</td>
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<td>4:50</td>
<td>Samantha Koutsares - Search for Higgs Bosons in Association with Top Quark Pairs decaying into Hadronic Taus</td>
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<td>5:03</td>
<td>Patrick Moran - Search for a Higgs-Top Quark Pairing in the Opposite-Charged Dilepton Channel</td>
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Poster Presentations Schedule
Jordan Galleria
12:00 noon – 2:00pm

Session I
12:30 - 1:00 pm

Thomas C. Adams - Project Based Learning, Polymer Membranes, and Ionic Liquids
Katherine Andreasen - Creating Multifunctional Semiconductor-Graphene-Metal / Quantum Rod Sensors on Flexible Substrate for the Detection of Aromatic Compounds
Kenisha Barber - Fabrication of Surface Enhanced Raman Scattering (SERS) Substrates using Gold Nanoparticles and Polymethyl methacrylate (PMMA)
Omar Beleh - An Irreversible Chemical Genetic Approach with c-Abl for use in Synergistic Studies
Janelle Biehl - Electrodeposition of Indium Thin Film Microwells for Preparation of Crystalline Indium Arsenide
Aryeh Blumenreich - Better Pathways in the Synthesis of Polymer Based Solar Cells
Caleb Bomske - Effect of Substrate on Transport of Corn Pollen in Streams at LEEF
David Boyer - Characteristics of Phenylacrylic Acid Decarboxylase (PAD) and Ferulic Acid Decarboxylase (FDC) in Saccharomyces cerevisiae
Tiffany Brocke - RFRP-1 ligand-receptor contacts in a model organism provide insight into cardiovascular physiology
Adam Buckner - Distinguishing between Disulfide Bonding Patterns in Antibody Structural Variants using Ion Mobility-Mass Spectrometry
Elija Buie - Analyzing the Social Determinants of Health Inequities using Data Mining Techniques
James Campbell - Detection of Environmental Coliphage Through Alpha-Complementation of Beta-Galactosidase in a Fast-Acting Bacterial-Based Biosensor
Rene Celis-Cordova - Ultra-Low Energy Microprocessor Design
Luis Cortes-Herrera - Design of a quasichaotic optical multipass cell
Nicholas Deason - Evaluation of outdoor insecticide-impregnated barriers, a new intervention for malaria control, in the Solomon Islands
Rose Doerfler - Thermal Stability of DNA Origami on Mica in Inert and Oxidative Environments
Sean Dwyer - Using the Natural Bond Orbitals of Ionic Liquids to Predict Relative CO₂ Binding Strength
Josephine Eshon - Mechanistic study of C(sp3)- Halogen Bond-Forming Reductive Elimination at Pd(IV) Centers
Mary Feng - Science Gateway Development for Vector-borne Diseases
Brad Ganoe - The Iterative Second-Order Green’s Function Method (GF2) for Electron Correlation
Tyler Gibson - Characterization of Anopheles gambiae G-protein coupled receptors as targets for novel insecticide development
Sebastian Gonzalez - Designing Primers for the parasite Blastocystis spp.
Brett Goodrich - Effect of Water on Physicochemical and Electrochemical Properties of Ionic Liquids Containing Aprotic Heterocyclic Anions
Jordan Gregory - Electrodeposition of reduced graphene oxide on metal oxide substrates: effect of loading on activity in heterogeneous Co(S2C6Cl2H2)2 dihydrogen production systems
Joseph Gurrentz - Heterogeneous cobaloxime dihydrogen production systems; systematic analysis of conjugated pyridine tethers for electrostatic adsorption to reduced graphene oxide
Allison Hendershot - AS-PCR as a Diagnostic for Differentiating Between Anopheles funestus Chromosomal Forms: Folonzo and Kiribina
Sara Hockney - Generation and Validation of a pax6b:GFP Transgenic Zebrafish Line
Qian Hou - Investigating the effects of osmolytes on the folding of the preQ1 riboswitch
Hillary Husband - Infrared spectroscopy studies of hydrogen-bonded clusters of ferrocene carboxylic acid (FcCOOH) in solution
Ana Illera Lopez - Effects of glucose and phosphorous limitation on growth and uptake kinetics of freshwater bacteria
Nirbhay Jain - A Simple Method of Minimizing Ionic Strength to Reduce Chemical Shift Variation in NMR-based Metabolomics of Urine Specimen
Sr Kanna - DASPOS: Data and Software Preservation for Open Science
John Kearns - Investigation of Thermal Rectification during Transient Heat Conduction
Andrea Kocher - Ultrafast Nonlinear Spectroscopy of Fluorescent Nuclear Chromophores
Claire Kozemchak - Synthesis, Characterization, and Reactivity of Non-Heme Iron Nitrosyl Complexes
Daniel Kwasnieski - Developing nitrile Stark probes of plasmonic fields
Qiuhan Li - New Avenues for Iron-Catalyzed Dehydrogenative Cross-Coupling Reactions
Darryl Lopez Velazquez - Study of peptides by incorporation of bromophenyl compounds using Suzuki Cross Coupling Reaction
Dara Marquez - Validating Paper Analytical Devices (PADs) using Metronidazole
China Mauck - A Model for Transport in Stereocilia
Rachel Miceli - Genetic analysis of podocyte development
Sneha Modi - Landscape and Anthropogenic Factors Drive Blastocystis Prevalence and Genetic Variation in Balinese Macaque Populations

Raquel Montanez-Gonzalez - Macaca fascicularis population structuring dictates distribution of genetic variation in Blastocystis across two islands in Southeast Asia.

Christina Na - Asymmetric, Metal-free Dihydroxylation Reaction using the Cyclic Peroxide of 1,1’-Binaphthyl-2,2’-dicarboxylic Acid

Sam O’Mahony - Non-Boolean computing using oscillators

Daniel Ocasio - Photostability Studies of Hydroxocobalamin

Alejandra Ortiz - Discovery and Validation of a Y-locus in Aedes aegypti and Determination of Polyandry

Sirisha Pasupuleti - The role of Scribble in epithelial cancer metastasis

Zhuoyu Peng - Speciation of Organic Compounds in Cloud Water from Whiteface Mountain

Sarah Philo - Classification of divalent cation effects on motility patterns of the bacterium Pseudomonas aeruginosa

Kenneth Poling - Hydrogen Production from Ammonia-Borane using Ruthenium as a catalyst

Samantha Rack - A System for Time Synchronized Data Capture for the Study of Joint Action

David Read - Exploring Diverse Functions of Mod5 and TRIT1

Federica Ricci - ULTRAFAST OPTICAL INVESTIGATIONS OF DIPOLAR AND QUADRUPOLAR MOLECULES OF THIOPHEN-2-YL PYRIDINIUM IODIDES WITH VINYL LINKAGES

Arianis Riofrío Díaz - Development of novel organometallic catalysts for the copolymerization of carbon dioxide and epoxides

Ann Rutherford - Development of novel organometallic catalysts for the copolymerization of carbon dioxide and epoxides

Natalie Sanders - Windows Azure as a Platform for Malaria Modeling

Megan Schutzbach - C-H Activation of a Common Intermediate for NF-κB Inhibitors

Sakshi Singh - Photo-Induced Frenel-Zone-Plates for Tunable Terahertz Beam Focusing

Barbara Slagel – Computational Periodic Trends of Catalysts for Methane to Methanol Conversion

Robert Stanley - Isolation of Antimicrobial Compounds from Red Oak (Quercus rubra L.) Acorns

Peter St George - Expression of notch1a and notch1b in the Light Damaged Zebrafish Retina

Gabrielle Thivierge - Determining the stage of diapause induction in Papilio glaucus

Fatima Ugur - Tuberculosis Drug Discovery: Mutagenesis Studies of the β’ subunit of Mycobacterium tuberculosis and Escherichia coli RNA Polymerase
Sierra Vanderkelen - Structure Based Functional Comparison of 3-deoxy-D-manno-oct-2ulosonic Acid Transferase

J. Garret Verwer - Optimizing the loading of FeOOH cocatalyst on WO₃ electrodes to improve pH stability and oxygen evolution efficiency

Jiarui Wang - Probing the effect of different ligands on the conformational dynamics of a transcriptionally acting preQ₁ riboswitch using single molecule FRET microscopy

Danielle Williams - Hsp70 and the Effects of XIAP Levels in Cancer Cells

Jenna Wilson - The Use of Fiducial Markers in Image Analysis

Yijun Xie - Connecting RomR Protein Dynamics in Myxobacteria to Polarity and Motility

Jeffrey Yu - Generation of TALEN-induced Aaop1 Knockout in *Ae. aegypti*

**Session II**

1:00 – 1:30 pm

Pauline Alokolaro - Polymer Nanofiber Fabrication

Slagel Barbara - Computational Periodic Trends of Catalysts for Methane to Methanol Conversion

Maximillian Baria - Surface Immobilization of AMPs Using Click Chemistry

Margaret Berta - The Physical Analysis of Kenyan Pharmaceuticals Aids in the Identification of Substandard Pharmaceuticals

Hannah Birky - Characterization of Genes that Govern Retinal Patterning in *Aedes aegypti*

Brenna Boehman - Probing the Interaction of Farnesyl pyrophosphate synthase by the IFN inducible protein Viperin

Buchanan Bourdon - Electrostatic Doping of 2D materials via Polymer Electrolytes: Using COMSOL to Simulate Ion-Electron Transport

Elena Brindley - Characterizing the Effect of Vitamin A Deprivation on *Aedes aegypti* Landing Behavior

Alexander Brown - Studying Disease Related Protein Aggregation Using Ion Mobility-Mass Spectrometry

Kendra Bufkin - Multimodal Imaging Trials with Zebrafish Specimens

Rose Calhoun - Mixed Matrix Membranes for Efficient Gas Separation

Anna Capote - Parents’ Caregiving History and Current Parenting Stress: A Comparison of Mothers and Fathers

Vanice Cheung - Supporting critical care teams with shared interactive displays

Bonnie Leigh Cruser - Screen to identify *Mycobacterium marinum* strains that are non-cytotoxic to amoeba
Joshua Dempsey - Biocomplexity and uncertainty: Science, technology, and ethics in the real-world case of silver nanoparticles in heavy commercial use

Eric Donahue - A Chemical Genetic Screen of the ICCB Known Bioactives Library and Exploration of the Peroxisome Proliferator-Activated Receptor (PPAR) Signaling Pathway During Nephrogenesis

Benjamin Elling - Shielding Effect of Plasma Treatment on Plasticized PVC Films during Microwave Exposure

Alvin Essenburg - GaN Vertical Junction Field-Effect Transistor for Energy-Efficient Power Conversion

Patrick Foley - Auto-prober I-V Measurements - How To Measure 100 Devices In 60 Minutes

John Gensic - A quantitative estimation of trap stiffness using a CMOS camera

Robert Gilson - Generating Induced Pluripotent Stem Cells from Adult Cancer Cells

Marangely Gonzalez-Cruz - Effect of dissolved oxygen on nitrous oxide (N2O) formation in biofilm systems for wastewater treatment

Ashley Graves - Dose Dependent Electrophysiological Responses to Yeast-Derived Volatile Compounds in Drosophila

Nathaniel Griggs - Development of Apparatus and Conditions for µPECVD of Nanodiamond

Kristy Hamlin - Single Molecule Techniques probing Spliceosomal Helicase Prp22

Madeline Herman - A Novel Tandem Pd-Catalyzed Carboamination/Diels-Alder Reaction

Peter Hoffman - Synthesis of a New Nickel (II) Complex

Meagan Hughes - The Impact of An Elevated Temperature and Projected Climate Change on L. melissa samuelis

Katherine Iliff - Cationic Gold Nanoparticle Contrast Agents for Detecting Damaged Cartilage and Tendon

John Jacobs - Characterization of matrix metalloproteinase-8 inhibitors for the treatment of sudden inflammatory response syndrome

John Johnstone - Adsorption Tuning in Graphene Oxide for the Design of Smart Materials

Micah Katz - Tandem Reversible Irreversible Cross-linking (TRIC): A Novel Method for Examining Localized Protein-Protein Interactions During Eukaryotic Gene Transcription

Darcy Kindelan - Water Filtration and Purification through Functional Nanofiltration Membranes

Jeff Kindelan - CO2 Capture Using Heterocyclic Molecules

Savannah Kounelis - Olfactory responses of a highly conserved Anopheles mosquito odorant receptor to plant odors
Wyatt Kuhlman - Synthesis of Targeted Polyethylene Glycol Nanoparticles for Cardiac Photodynamic Ablation Therapy

David Lawrence - Catalytic Fast Pyrolysis of Lignocellulosic Biomass with Manganese-Incorporated MFI & MTW Zeolite Catalysts

Keenan Linder - Thermal Stability of DNA Origami Bonded to APTES Monolayers and Silicon Surfaces

Desmond Madu - Chemical Composition Analysis of Rainwater Collected in Ann Arbor, Michigan

Michael Martinez - A Patient Simulator Control System for Clinical Operators

Rory McAtee - Visible-Light Mediated Synthesis of Constrained Cyclic-Peptides from Phenacyl Protected Cysteine Residues

Pierre Alexander Miranda Herrera - Stability of the solar cell absorber methylammonium lead iodide perovskite during exposure in humidified air

Christina Monnie - *In vitro* modification of bacterial peptides by mammalian prenyltransferases

Brenda Mueller - Germanium Semiconductor Testing: Using a Photo-luminescence System

Eva Niklinska - Actin-mediated IKNM in Regenerating Adult Zebrafish Retina

Katie O'Neill - Depositing and characterizing two-dimensional electrolytes for low-voltage memory

Akwasi Opoku - Development of Paper-based Electrochemical Measurements for Biosensing

Stephanie Pastrana - Production and Purification of P.69T 2K for mimicking its secretion through its own translocator domain

JaMarcus Payton - Inhibition of MMP-12 and ADAM10 by DR-04-086

Steven Penny - Artificial Tissue Formation Using Laser-Based Optical Tweezers

Samantha Piekos - Characterization of rod precursor proliferation in the dark adapted, adult zebrafish retina

Jamon Pulliam - The Effect of a Summer Robotics Camp on Social interactions for Adolescents with Autism Spectrum Disorder

Christian Ramsland - Studies of a Semi-Water Soluble non-heme FNOR Model Complex

Barry Reid - Material characterisation of hybrid organic/inorganic perovskites for solar cell applications.

Tabitha Ricketts - Qualitative Computational Analysis of Paper Analytical Devices

Colleen Riordan - Surface-enhanced Raman detection of carbohydrates

Katherine Sanders - Stochastic computing and nanomagnet logic (NML)

Siddharth Saraph - Mobile Device Network Traffic Capture and Analysis

Abigail Shepard - Blinded by the Light: A Vitamin B<sub>12</sub> Kinetics and Quantum Yield Study
Ryan Soheim - Modification of Curcuminoids and Studies on their Modes of Action
Tony Stedge - Development of an Anatomic Human Breast Imaging Phantom for Investigating Contrast-Enhanced Detection of Microcalcifications
Denise Tarnowski - Synthesis of N-glycosylated Cetuximab in *Bombyx mori*
Diamond Thomas - Reactivity of cobalt(II) tetraphenylporphyrin complexes with nitrosoalkane compounds
Megan van der Horst - Synthetic Pathway towards Functionalized TMP Dendritic Conjugates for Malaria Enzyme Targeting
Ricardo Javier Vazquez - Ultrafast Time-resolved Spectroscopy of Donor-Acceptor Photovoltaic Copolymers Based on 2,6-di(thiophen-2-yl)benzo[1,2-b:4,5-b’]difuran
Justin Waller - Maximum Constraints of Resolution Detected in Planar (Xtreme) & Computed Tomographic (CT) X-ray Modalities
Michael Weber - Effects of open water leads in sea ice on Arctic snow chemistry
Russell Williams III - Exploring Proteinase-activated Receptor-2 (PAR2) Mediated p65/p50 Canonical Pathway Activation in Oral Squamous Cell Carcinoma
Mark Wilson - Photovoltaics: Cu$_2$S Synthesis, Solar Cell Efficiencies, and Applications
Brandon Yik - Energy Storage Devices with Organic/Hybrid Macromolecular Materials
Wuliang Zhang - Molecular Characterization of Dissolved Organic Matter in Cloud Water from Whiteface Mountain (NY)
ABSTRACTS
Oral Presentation

*Characterization of thin foils as target materials for nuclear reactions*

Luis AbregoRangel  
Advisors: Ani Aprahamian and Khachatur Manukyan,  
Dept. of Physics, University of Notre Dame

An accurate measurement of thickness of targets is crucial for the study of nuclear reactions, specifically in determining the absolute cross section for a given reaction. Existing methods show some strengths and limitations. One of the most standard ways of measuring target thickness is by the loss of energy of alpha particles produced by an accelerator. My project this summer was focused on introducing a new method from material science to measure target thicknesses. We focused on the application of an ion beam coupled to a scanning electron microscope (FIB/SEM). This instrument has taken its place in several fields as a standard method due to its versatility to characterizing materials with high resolution, here we apply it to a more precise determination of target thickness to use in reducing the errors in measuring nuclear cross sections due to target thickness. Focused ion beam instrument from the Notre Dame Integrated Imaging Facility (NDIIF: a general facility available in the colleges of Engineering and Science at ND) is used to determine the geometrical thickness of thin self-supporting film targets. We compared thicknesses obtained by energy loss measurements of alpha particles from a radioactive source with energies of 3.183 MeV ($^{154}$Gd) and 5.486 MeV ($^{24}$Am); discrepancies will be discussed with the energy loss method. Future investigations include comparisons with Rutherford scattering and the use of well known resonances.
Renewable energies such as wind and solar are possible alternatives to carbon-based sources of energy. However, both wind and solar cannot continuously generate enough energy to meet the world’s current needs. They are limited by weather conditions and daylight itself. Therefore, it would be necessary to store energy in large quantities. Current battery designs for such a large scale are costly, and in some cases may not be safe. Consider lithium ion batteries that have electrolyte solutions that may be flammable under certain conditions. One alternative might be an Ionic Liquid electrolyte solution, which is not flammable. However, to combat the dendrite growth that is commonly found in lithium ion batteries one might implore permeable polymer membranes. These membranes must have hole diameters large enough to permit lithium ions to pass, but small enough to prohibit dendrite growth, which can cause short circuits and lead to fires. Current research shows that soaking these membranes in various solvents can impact swelling and change diameter sizes. My research attempts to identify characteristics of ionic liquids that might serve as predictors of these effects. I have calculated the Kamlet-Taft values to determine the ionic liquids hydrogen bonding donor / acceptor scales as well as the dipolarity / polarizibility ratios, and compared them to polymers soaked in the corresponding ionic liquids to see if these values have any correlation to membrane swelling effects.

In addition, I am also charged with the task of using data from this research to teach the Next Generation Science Standards in Engineering Design to my high school students. My unit plan walks my students through each step of my research while teaching them content standards from chemistry, physics, mathematics, and engineering. Their main objective is to relate content area concepts to their application in the real world – especially the ionic liquid research at the University of Notre Dame’s Department of Chemical and Biomolecular Engineering.
Polymer Nanofiber Fabrication

Pauline Alokolaro
Tengfei Luo
Teng Zhang
Advisor: Tengfei Luo, Dept. of Aerospace and Mechanical Engineering,
University of Notre Dame

Polymers are inexpensive, lightweight and durable. In addition, amorphous polymers are both electrically and thermally insulating. For this reason, they are ideal for use in manufacturing. Polyethylene has shown promise as a thermal conductor when converted from its amorphous state to its stretched state making it more versatile for use as an alternative in the fabrication of micro- and nanodevices among other uses. Theoretical calculations suggest that the thermal conductivity could be higher than some pure metals—orders of magnitude higher than the thermal conductivity of amorphous polyethylene making it useful in thermal transport systems. A polymer gel was synthesized and then disentangled. Diameter of resulting chains was observed using a microscope. The experience will be incorporated into a high school geometry class during a unit involving the surface area and volume of solids. Students will be given one solid and a jar and asked to calculate how many congruent solids will fit in the jar. They will confirm their theoretical findings experimentally by filling the jar with congruent solids. As an extension, students will be given a quantity of solids and asked to choose or design the best container. Discussions of packaging and waste will be part of the activity.
Titanium dioxide coupled with graphene oxide nanosheets provides a platform to photocatalytically deposit silver nanoparticles and create semiconductor–graphene oxide–metal (SGM) films that are capable of detecting and degrading organic toxins. 2-D graphene oxide nanosheets can be used to concentrate target molecules for sensing applications. Reduced graphene oxide has also been used to ease electron transfer through layers of CdSe/CdS quantum dots because of its electronic transport properties. We are designing and constructing sensing strips composed of titanium dioxide, graphene oxide, and silver nanoparticles on a conducting, flexible plastic substrate. In this project, we are combining these properties to design multifunctional patterned sensing films useful for quick response detection and degradation of aromatic compound on the flexible substrate. The feasibility of this approach is being tested with crystal violet and nitrobenzene as a target molecule. Raman, ultraviolet visible, and emission spectroscopy are being used for sensing the presence of crystal violet and nitrobenzene on the films. Decomposition of nitrobenzene to aminobenzene using these sense and shoot strips has been demonstrated under visible light irradiation.
Fabrication of Surface Enhanced Raman Scattering (SERS) Substrates using Gold Nanoparticles and Polymethyl methacrylate (PMMA)

Kenisha Barber
Advisor: Zachary Schultz, Dept. of Chemistry and Biochemistry, University of Notre Dame

Raman Spectroscopy is a nondestructive way to provide chemically specific information on individual molecules; however, it has poor sensitivity. To improve or increase these Raman signals, Surface Enhanced Raman Scattering (SERS) can be used. SERS occurs when surface plasmons from metals are excited by incident light. This excitation can enhance the Raman scattering by $10^{10}$. A SERS substrate was fabricated by assembling a film of gold nanoparticles onto a support. Gold nanoparticles were synthesized from hydrogen tetrachloroaurate (III) trihydrate and sodium citrate. The SERS substrate was fabricated using the gold nanoparticles, a PMMA in toluene solution, and ethanol that was slowly added. With the addition of the ethanol, the gold nanoparticles rose to the toluene/water layer while a thin PMMA film formed on top. Upon evaporation of the toluene, the gold nanoparticles were captured in the PMMA film and then placed onto glass or plastic support. The substrate was allowed to dry under vacuum and low heat. To assess the SERS enhancement, the Raman scattering from the thiol, 4-mercaptobenzonitrile (mbn) was measured. Raman spectra were obtained using the Renishaw microscope and laser (633nm) system. The effectiveness of the substrate for SERS activity was compared on the glass, both front and back, and on the plastic media. The substrate on glass showed better enhancement than on the plastic. This substrate shows to have good potential for SERS applications because of its optical transparency and high SERS activity. It is also simple to fabricate.
Antimicrobial peptides (AMPs) are a rising topic within research. Compared to antibiotics, AMPs are less likely to develop bacterial resistance. Surface immobilization has been widely used in biochips and biosensors. In this study, AMPs with an azide mutation at different terminus were applied using “click chemistry” for immobilization with alkyne terminated abiotic surfaces. Click chemistry forms a triazole linker, when an alkyne and an azide interact with each other to induce immobilization. Surface immobilization of AMPs was monitored via contact angle to determine the surface characteristics of the alkyne functionalized surface and circular dichroism (CD) determined the abundance of the \( \alpha \)-helix and secondary structures of immobilized AMPs. Contact angle results indicated that the alkyne was functionalized on the surface and CD results presented that during surface immobilization the \( \alpha \)-helix and secondary structures were protected in the process. This research provides further insight into characterization of surface immobilized biomacromolecules.
Protein kinases have become important drug targets due to their involvement in many biological processes, including cell division, motility, and overall survival. Dysregulation of these signaling molecules has been shown to lead to disease, particularly in a number of different cancers. Previous research has led to the development of ATP-competitive inhibitors that effectively target multiple kinases. However, this approach has only been proven to be successful in a limited number of disease treatments. A lack of cellular potency and selectivity has limited the utility of single agent dosing regimens for kinase inhibitors, as there are over 500 kinases in the human genome. One approach to improve treatment of dysregulated kinases is combination therapy, which involves the use of multiple drugs to treat a single disease. Here we report the design of an irreversible chemical genetic approach with c-Abl through the synthesis of an irreversible analog of GNF-2, a known allosteric inhibitor of the kinase. This inhibitor will bind to the kinase’s myristate pocket and covalently label an inserted cysteine residue within the site. Through biochemical binding assays, synergistic studies will be run to examine the effects of permanent binding to the myristate pocket of c-Abl has on known ATP-pocket binders.
Poster Presentation

*The Physical Analysis of Kenyan Pharmaceuticals Aids in the Identification of Substandard Pharmaceuticals*

Margaret Berta  
Rebecca Ryan  
Steven Froelich  
Advisor: Marya Lieberman, Dept. of Chemistry and Biochemistry, University of Notre Dame

In many developing nations counterfeit and substandard pharmaceuticals pose a serious and widespread problem. Often manufacturers of substandard pharmaceuticals are not only negligent with the ingredients in the drugs they produce but also in the packaging of the product. If low quality pharmaceuticals were able to be identified by the physical characteristics of the packaging and tablet or capsule, this would provide more assurance of the PADs test result. A physical forensic analysis of over 400 packages of pharmaceuticals was conducted. I wrote a list of criteria for specific characteristics of the tablet/capsule, which were rated as either a pass or fail for the initial physical analysis. For example, tablets that were moldy or crumbling and capsules that were dented or had illegibly printed markings were rated as failing. The Kenya Pharmacy and Poisons Board, 2012 and 2014 Drug Registration Databases were used to determine registration of brands and manufacturers. Overall, 26% of amoxicillin samples, 1.92% of amoxyclav samples, 1% of the ciprofloxacin samples, 7.07% of azithromycin, and 19.48% of paracetamol samples failed physical analysis. In total, 146 samples, 33.72%, were not registered on the KPPB database. The samples from one brand failed 100% of the physical analyses and were not listed as registered in the KPPB online database. The physical analysis and registration status were then compared to HPLC results of a subset of the samples. Overall, physical analysis and manufacturer registration were effective in identifying low quality pharmaceuticals. Failure to meet simple physical criteria not only suggests that a particular pharmaceutical could be low quality, but also identifies manufacturers that produce drugs that may not meet standard chemical specifications.
Through a new electrochemically-gated alloying reaction scheme, Indium (In) thin films can be readily transformed into thin InAs films. Microfabricated arrays of $10 \times 10 \, \mu\text{m}$ wells in both negative (SU8 2007) and positive (AZ9260) photoresist ($t = 10 \, \mu\text{m}$) were prepared. Indium thin film microwells were prepared at room temperature by electrochemically reducing InCl$_3$ on micropatterned n$^+$-Si(100) electrodes in acidic electrolytes. Constant current and constant potential conditions, along with bath composition, and precursor identity were evaluated to identify conditions where the In film Rrms roughness was minimized and thickness control was maintained. Subsequent electrochemically-induced alloying of the In thin film microwells directly to crystalline InAs was confirmed by Raman spectroscopy after electrochemical reduction of dissolved As$_2$O$_3$ at the In micowell sites. Further, lift-off of the SU8 resist was studied to identify conditions where free-standing InAs microstructures could be fabricated. Electrodeposition of In thin film microwells followed by direct preparation of crystalline InAs is a promising alternative approach for future preparation of larger In/InAs thin film deposits.
Studying the visual system of the *Aedes aegypti* mosquito could provide novel avenues for vector control and disease transmission intervention, including the creation of visual mutants and improved mosquito traps involving visual cues. The *Aedes aegypti* retina is composed of four distinct regions—the dorsal, central, ventral stripe, and ventral regions—distinguished by the rhodopsins expressed in the R7 photoreceptor cells. This study examines the expression of transcription factors governing this retinal patterning. Five transcription factors, homothorax (Hth), Iroquois complex (IRO-C), wingless (wg), orthodenticle (otd), and spineless (ss), were chosen to study because they are known to determine cell fate in *Drosophila* by specifying which rhodopsin is expressed in each photoreceptor cell. The current study examines these transcription factors in adult *Aedes aegypti* using in situ hybridization, modeled from the protocol for zebra fish embryos. A 200-400 base pair region of each gene was PCR amplified and cloned into the TOPO2.1 vector. An EcoR1 cut was used to check for the presence of the insert in the plasmid vector. After a series of minipreps and midipreps, the plasmid was linearized with a BamH1 cut. The linearized DNA was then purified and used to make digoxigenin (DIG)-labeled RNA probes. Heads from white-eyed *Aedes aegypti* one to four days post-eclosion were fixed, and then whole mount retinas were dissected before being treated with the DIG RNA probes. The probes were detected in the retinas with an anti-DIG antibody conjugated to alkaline phosphatase and colorimetric (NBT and BCIP) substrates. When a stain appeared on the retinas, they were then mounted and imaged with a light microscope. This study will shed light on the genetic basis for retinal patterning in *Aedes aegypti* and open doors to create and study visual mutants, ultimately for the purpose of contributing to vector control efforts.
Solar power is a rapidly growing source of renewable energy. While silica cells currently provide a relatively high level of efficiency, carbon based solar cells, particularly conjugated polymers, also show promise as an alternative material for a solar cell. The chain-growth method has proven to be an effective way of making conjugated polymers, providing control over polymer length, sequence, and end groups. However, this method currently only works well with a small number of monomers. As such, there is considerable interest in extending the chain-growth method to the polymerization of monomers with a wider range of properties. Biaryl monomers, in particular, have shown promise as a new method to create better solar cells and have several benefits over simple heterocyclic monomers. For example, they offer increased control over polymer properties, such as solubility, absorption, or effective conjugation length, by varying the aryl species involved in the monomer. Significantly, polymers with perfectly alternating sequences offer a uniform conduction band and absorption spectrum, crucial properties for making polymer based solar cells. While alternating sequence polymers are commonly accessible in other methods of polymerization such as step growth, the chain growth method provides even greater control over polymer properties. However, poly(2-(2,5-bis(2-ethylhexyloxy)phenyl)-thiophene) is the only reported example of a polymer composed of a biaryl monomer synthesized by the chain growth method. In order to show that having a biaryl monomer is feasible, it is necessary to first reproduce this result. If this is successful, it is much more likely that other alternating biaryl polymers can be synthesized as well, extending the benefits of a biaryl system to a wider array of polymers.
Probing the Interaction of Farnesyl pyrophosphate synthase by the IFN inducible protein Viperin

Brenna Boehman
Gabriel Román

Advisor: Neil Marsh, Dept. of Department of Chemistry, University of Michigan

Viperin (Virus Inhibitory Protein; Endoplasmic Reticulum associated, INterferon inducible) is an interferon stimulated gene which is shown to have direct antiviral activity against a number of pathogens that infect eukaryotic cellular based organisms. Sequence analysis reveals a CX3CX2C iron-sulfur cluster binding motif suggesting Viperin belongs to the ever-growing radical S-adenosylmethione (SAM) family group of enzymes. The iron-sulfur cluster chelates SAM and these enzyme are then able to generate a highly reactive 5’-deoxyadenosyl (5’dA) radical intermediate via reductive cleavage of SAM’s 5’-C-S bond. The 5’dA radical is then used to generate a wide variety of challenging chemical transformations.

Farnesyl pyrophosphate synthase (FPPS), a key enzyme in the mevalonate pathway along the way to cholesterol biosynthesis, is an established target for viperin and our goal is to understand the basis for their demonstrated interaction, as well as the role radical-SAM chemistry may play in the reported inhibition of FPPS. We have cloned both viperin and FPPS in pcDNA3 series vectors with a FLAG and HIS epitope tag respectively, allowing each protein to be independently detected. Using the CMV promoter to drive expression allows us to use the HEK293T cell line and provide a system that is physiologically relevant in which to probe the activity of viperin as well as its interaction with FPPS.
Substrate affects the concentration and transport rate of environmental DNA in streams. The ability of a stream to retain environmental DNA (eDNA) is largely dependent on the composition of the substrate. We conducted our experiment at the University of Notre Dame’s innovative Linked Experimental Ecosystem Facility (LEEF) at St. Patrick’s County Park, and used corn pollen as an FPOM substitute to mimic the movement of eDNA in a stream. At LEEF, semi-natural streams mimic the movement and flow of natural streams. We used four types of substrate for comparison in each of the four streams including pea gravel, cobblestone, a 50/50 mixture of pea gravel and cobblestone, and an alternating pattern of two meters of pea gravel to two meters of cobblestone. The corn pollen was pulse-released in each of the four streams. We monitored concentration fluctuations of the corn pollen at four sites along the 50-meter reach of the stream, ten meters apart to capture the pulse of corn pollen as it dispersed downstream. Results suggest that pea gravel has a higher retention of corn pollen than cobble, with the mixed and alternating substrate intermediate between the two. Therefore, finer substrates retain more corn pollen than course ones. The relationships demonstrated by this experiment are vital to a comprehensive understanding of eDNA source location in streams.
As electronic devices become smaller, the need for low-power components increases. Two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides (TMDs), are promising because they allow us to approach the limits of vertical scaling when integrated into devices. However, new doping strategies are required for 2D materials because traditional strategies, such as substitutional doping, will destroy the electrical properties of the materials. One strategy is electrostatic doping using ions. In our lab, we use ion doping to modulate the electrical conductivity of a graphene channel for the development of a new, 2D memory device, and to create p-n junctions for tunneling in 2D field-effect transistors (FETs). The goal of this summer’s research was to use COMSOL Multiphysics Software to model ion-electron transport to better understand the underlying fundamental physics of electrostatic doping, and inform the experimental approach. To simulate the formation of the electrostatic double-layer required to increase the current through the graphene, we modeled a 100 × 100 nm parallel-plate device consisting of graphene / polymer electrolyte / graphene, where the polymer electrolyte was polyethylene oxide (PEO) and LiClO₄. Using materials properties derived from experiment, including dielectric constants and ion diffusion coefficients, we described ion transport by coupling the Nernst-Planck equation with Poisson’s equation. We determined that in the 100 × 100 nm parallel-plate model, with an applied electric field of 1 mV/nm, the ions establish an electrostatic double-layer in 0.5 s, and relax to equilibrium in 1 s at room temperature. We studied dynamic p and n-type doping by sweeping the gate voltage (V_G) between ±150 mV and monitoring the cation (Li⁺) and anion (ClO₄⁻) charge carrier density at the graphene surface. From experiment, we know that if the V_G is modulated by 0.2 V/s, the ions will not have sufficient time to reach equilibrium, giving rise to a large hysteresis in the current-voltage (I_d-V_G) data (Fig. 1). This result is qualitatively captured by the COMSOL simulations (Fig. 2). When the sweep rate is decreased from 1 V/s to 0.01 V/s, the ions have sufficient time to reach steady-state and exhibit no hysteresis (Fig. 2).
The environmental, economic, and geopolitical concerns over continued fossil-fuel dependence has spurred research into the manufacture of renewable and sustainable petroleum-based chemicals. One of the most prominent methods to accomplish this goal is the \textit{in vivo} production of non-natural metabolites via a combination of metabolic engineering, systems biology, and synthetic biology. This process is greatly benefited by detailed knowledge of the mechanism of the related enzymes. Here, we are interested in better understanding ferulic acid decarboxylase (FDC) and phenylacrylic acid decarboxylase 1 (PAD1) from \textit{S. cerevisiae}, which are involved in the decarboxylation of phenylacrylic acids to produce styrene, 1,3 pentadiene, 4-vinylphenol, and 4-vinylguaiacol. These products are commercially valuable and have potential applications in the biosynthetic production of a variety of valuable chemicals including polymers, biofuels, and industrial flavoring. Also, this reaction might present a novel decarboxylase mechanism. Our previous study showed that PAD1 makes an unknown cofactor to activate FDC in order to decarboxylate trans-cinnamic acid, our model substrate, and produce styrene. Here, we have constructed several \textit{E. coli} strains in order to express these proteins in both their active and inactive forms so that we may simultaneously attempt to reconstitute the system \textit{in vitro} and to isolate the cofactor from the holoenzyme. This allows us to both understand conditions necessary for cofactor production and to investigate the identity of the cofactor isolated from the holoenzyme. In order to learn more about these enzymes and identify their cofactor, we have conducted a variety of bioanalytical techniques including GC-MS, LC-MS, HPLC, H-NMR, Native PAGE, SDS-PAGE, among others. Our research results could serve as bases for engineering efforts on FDC and PAD, which might ultimately lead to microbial cell factories capable of producing sustainable and valuable chemicals.
Poster Presentation

**Characterizing the Effect of Vitamin A Deprivation on Aedes aegypti Landing Behavior**

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Matthew Leming and Michelle Whaley  
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*Aedes aegypti* mosquitoes are the primary vector for Dengue fever, a disease that affects almost 400 million people each year and has no known effective treatment or vaccine. Current vector control methods have failed at halting the geographic spread of this disease, emphasizing the need for continued research in vector behavior and control. Aaop1, the rhodopsin expressed in *Aedes aegypti* R1-R6 photoreceptor cells, reaches its final mature conformation in dark conditions and is then able to enter the rhabdomere and initiate phototransduction. The goal of the current study is to rear white-eyed *Aedes aegypti* on a vitamin A deprived diet of heart powder and examine the effects of this deprivation on Aaop1 maturation, Aaop1 levels, and landing behavior. Western blot results show that rearing on heart powder decreases overall Aaop1 levels by up to 16%. The heart powder diet also potentially inhibits the maturation of Aaop1, with only the larger immature form present in vitamin A deprived animals, preventing this crucial rhodopsin from entering the rhabdomere and acting in phototransduction. In order to link this rhodopsin impairment with landing behavior, a protocol was developed to measure landing preference between black and white landing surfaces using wild type of both the white-eyed and Orlando strains of *Aedes aegypti* to explore the behavior of animals with different eye pigmentation. Interestingly, the white-eyed preferred the white surface, while the Orlando strain preferred the black surface. The demonstration of distinct landing preferences by strain indicates that retinal pigmentation may play a role in the landing decision and also confirms the validity of the assay to discern varying preferences. These behavioral results will be compared to those of the vitamin A deprived stock, revealing the effects of rhodopsin impairment on landing preference. Observing a change in landing behavior as a result of visual impairment would assert the crucial role of the visual system in landing behavior related to vector host-seeking, opening opportunities for vision-focused vector control innovations.
Numerous physiological processes are mediated by peptidergic signaling through G-protein 
coupled receptors (GPCRs). Human RFamide-related peptide-1 (hRFRP-1; MPHSFANLPLRF- 
NH2) acts through neuropeptide FF receptor 2 (NPFFR2) to decrease cardiac contractility, but 
this pathway remains relatively uncharacterized. Identification of ligand-receptor interactions 
provides insight into which residues are critical for binding to the GPCR and activating the 
signaling pathway. Thus, these data contribute to a long-term goal of targeting cardiovascular 
physiology. We investigated RFRP-1 signaling in zebrafish, Danio rerio, a vertebrate model 
for human cardiovascular physiology. We predicted and established the presence of zebrafish 
RFRP-1 (zRFRP-1; PAHLHANLPLRF-NH2) and NPFFR2 transcripts in brain and heart. Next, 
we confirmed that zRFRP-1 decreased zebrafish cardiac contractility and LPLRF-NH2 and 
LPLAF-NH2 acted as an agonist and antagonist, respectively. I tested our hypothesis that zRFRP- 
1 interacted with zNPFFR2. We found that a salt bridge between R11 of the ligand and D106 on 
transmembrane helix 2 of the receptor was present in each cardioinhibitory peptide and absent in 
the antagonist. Our zRFRP-1 structure-activity relationship data also indicated that in zebrafish 
hRFRP-1 is more cardioinhibitory than zRFRP-1, thus, both ligands were docked to zNPFFR2 to 
gain insight into contact sites related to agonism. We found that F5 of hRFRP-1, a residue not 
present in zRFRP-1, makes a strong pi-stack to Y299 on TM7, an interaction not made by 
zRFRP-1. These discoveries in zebrafish begin to provide a basis for understanding RFRP-1- 
NPFFR2 interactions involved in cardiac contractility.
Poster Presentation

*Studying Disease Related Protein Aggregation Using Ion Mobility-Mass Spectrometry*

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Measurements combining mass spectrometry (MS) with ion mobility (IM) separation have shown that the quaternary structures of large protein aggregates can be largely retained in the absence of bulk solvents, thus enabling structural models of transient, disease-associated protein complexes [1-3]. IM separates ions based on their ability to traverse a chamber filled with inert gas under the influence of a weak electric field. Ion size in the form of an orientationally-average collision cross-section (CCS) is the primary information content of IM separation and established computational approaches can be used with this information to assign the structure of biomolecules. IM-MS is capable of making accurate measurements of structures and stoichiometries of intact multiprotein complexes at very low concentrations (µM) and within complex mixtures.

Protein aggregation has long been attributed to the etiology of many neurodegenerative diseases such as Parkinson’s, and more recently, protein aggregation has also been linked to cancer. Here, we describe our recent efforts to build IM-MS protocols to better understand disease related protein aggregation. Specifically, we will discuss the aggregation properties of the tumor antigen protein tetramer p53, as well as copper-related Ubiquitin aggregation linked to Lewy body formation associated with dementia. We use MS measurements to confirm the stoichiometry of complexes detected and IM to separate species with similar mass to charge ratios, while also allowing for the measurement of aggregate CCS. We will also discuss emerging measurements of protein-protein interaction strength, protein dynamics, aggregate topology models, as well as the development of new bioinformatic tools capable of detailed IM-MS data analysis.

Pharmaceutical companies develop antibodies for both research applications and as biotherapeutics. Antibody-antigen interactions can be very specific, and often driven by subtle differences in amino acid sequence, or in the number and pattern of the different disulfide bonds found within the intact antibody structure. Since antibodies are large (~150 kDa), a key challenge has been to develop analytical technologies capable of rapidly assessing their structures following production, as minor deviations can dramatically influence specificity and/or efficacy. Previous data from our lab has suggested that Ion Mobility-Mass Spectrometry (IM-MS) techniques could be viable for distinguishing antibody variants. IM-MS works by separating protein ions produced by electrospray ionization (ESI), first according to their orientationally-averaged size, and subsequently by their mass-to-charge (m/z) ratio. Since critically-important antibody structure variants can differ by less than 1% in their overall size, we have developed new IM-MS approaches to resolve such subtle differences. Our IM-MS antibody analysis approach selects a single charge state produced for intact antibodies produced by ESI, traps selected ions and subjects them to collisional heating in the gas phase. Once heated, antibodies unfold to reveal unique patterns, which we treat as ‘fingerprints’ that enable us to differentiate the number and patterns of inter-disulfide bonds within a variety of known antibody structures. In this presentation we will present data that demonstrates the capability of IM-MS to rapidly distinguish between these different forms. In the future, we aim to develop quantitative methods for developing distinct unfolding signatures of each variant. This information could be used to develop quality control procedures for pharmaceutical companies for determining purity of their antibody products and possibly as a method for studying next-generation biotherapeutics.
Biomedical imaging is an important technique that can be used for several applications such as cancer research and cardiology. A range of imaging technology, such as PET, SPECT, micro-CT and optical X-ray, is available for imaging. However, many research institutes use rats and mice for preclinical experiments. The purpose of this study is to determine if Zebrafish are compatible for use in pre-clinical imaging, and which modalities and probes work best. Different Zebrafish specimens were tested using four different modalities, and four probes. In order to assess with two-dimensional modalities, both fluorescence and planar X-Ray were performed on the specimens. The fluorescence imaging was acquire using OsteoSense 750x and ProSense 750x as the probes. Through the results, we discovered that OsteoSense did not work as well as the ProSense. The next two modalities represented three-dimensional imaging. These modalities consist of X-ray Computed Tomography (CT) and Positron Emission Tomography (PET). Sodium Fluoride (NaF), Fludeoxyglucose (FDG) were the two probes tested with PET imaging. The majority of the probes were detected in the specimens but not at the correct target.
Poster Presentation

*Analyzing the Social Determinants of Health Inequities using Data Mining Techniques*

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Authors and Affiliations: Dr. Nitesh Chawla  Waldo Mikels-Carrasco  Keith Feldman  Elija Buie

Social circumstances can have both beneficial and detrimental effects on the health of individuals. Access to healthy food options, local parks and recreational fitness centers are all factors that need to be considered when regarding the health and wellbeing of a community. The collection of data regarding these aspects provides substantial insight into diseases and ailments that appear to affect specific communities and provide a means of reducing and mitigating these risks.

In order to obtain the data around community health and wellness, we implemented a web crawler, which scours the Internet based on a list of keywords in order to find databases that contain relevant data. These databases, such as census data, typically obtain elements specific to Indiana, from which data from St. Joseph County is extracted. The emphasis is placed on St. Joseph County in order foster a deeper connection to the work as well as to demonstrate the effectiveness of social data in our own backyard.

Once the data is obtained it is then placed on a map in order to determine which areas are “hotspots” for diseases like obesity and diabetes. With visual representation highlighting problem areas, issues such as a lack of grocery stores or pharmacies can be addressed. By determining areas that are most susceptible to specific diseases, local clinics and health care centers can be catered to those diseases in order to reduce and prevent their occurrence in that area. Utilizing this social data could have significant effects not just on the county level but for the nation as a whole.
The TWINSOL facility at the Nuclear Science Laboratory of the University of Notre Dame can produce various kinds of low-energy light radioactive beams, including nuclei that beta decay to their mirror neighbour. Decay spectroscopy of such mirror transitions in ion traps can provide valuable information to test the electroweak interaction. However, the energy of the TWINSOL beams is not low enough to be used in trapping experiments. The typical method used at other facilities to produce very low-energy radioactive beams consists in slowing down the energetic beam using a gas cell. Such systems include a solid degrader to slow the beam down, an He-filled gas volume to thermalize the ions and a radiofrequency carpet to extract the ions of the device. Simulations of stopping and extraction of ions were made considering the characteristics of the radioactive beams that TWINSOL can produce. A preliminary design of the stopping station is presented according with the obtained results.
Poster Presentation

Mixed Matrix Membranes for Efficient Gas Separation

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In the U.S., 4,500 trillion Btu of energy, or about 22% of all power plant output, is used to separate industrial gases. Using polymer (plastic) membranes to separate those gases would require much less energy. Additional benefits of polymer membranes include low cost, a compact design with no moving parts, and low environmental impact. Triptycene-containing polyimides are an interesting new group of polymers. The unique 3-D shape of the triptycene molecule, consisting of three “blades” protruding from a single hinge, creates high amounts of space throughout the polymer, which leads to good gas separation properties. Mixed matrix membranes (MMMs) are polymer membranes that have inorganic fillers dispersed throughout. MMMs are easier to process and manufacture than inorganic membranes and are expected to have increased gas separation properties compared to polymer membranes. Zeolites are crystalline molecules made up of silicon, aluminum, and oxygen and are very good at absorbing small molecules. They are used in pet litter, wastewater treatment, detergent, for water purification, and are one type of inorganic filler added to MMMs. Another type of filler is metal organic frameworks (MOFs). MOFs are hybrids of organic and inorganic materials that have properties similar to zeolites, but they can be “tuned” to certain pore sizes, and they have better affinity for polymers. In this investigation, MMMs were produced by mixing the triptycene-containing polyimide, 1,4-triptycene para-6FDA, with varying amounts of zeolite 4A and zeolite ZSM-5. The films were imaged using scanning electron microscopy (SEM) to observe the distribution of the particles in the membrane and the interaction between the zeolite and the polymer. Preliminary findings suggest some void space between the particles and the polymer that could decrease gas separation performance, which will be investigated further with gas permeation measurements. Additionally, the films were tested using thermal gravimetric analysis (TGA) and found to be very thermally stable, breaking down around 500°C. Along with the zeolite work, a metal organic framework (MOF), called ZIF-90 was also synthesized to be incorporated into future MMMs. Testing of the ZIF-90 particles are in progress.
Detection of Environmental Coliphage Through Alpha-Complementation of Beta-Galactosidase in a Fast-Acting Bacterial-Based Biosensor.

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Judah Easton
Christopher Freitag
Vera Marcello
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Advisor: George Twaddle and Christina Arisio, Program for Nanotechnology, Ivy Tech
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The American Public Health Assay (APHA) for human waste contaminated water is hampered by a dependency on culturing coliform bacteria with a turn-around time exceeding one day. An assay for coliphage detection, as surrogate for coliforms, has been developed which employs the release of the host indicator cell beta-galactosidase enzyme activity by lytic coliphage and the conversion of a colorimetric substrate. While significantly shortening the APHA time to 3 hrs., this assay requires a laboratory equipment to separate phage-induced released β-gal enzyme from intact cells before addition of the substrate. To optimize this assay we have taken advantage of the α-complementation feature of beta-galactosidase. We are engineering cell lines containing either the gene fragments of LacZalpha for purification and will use an E.coli cell line with the M15 mutation expressing the omega fragment of Beta-galactosidase. We predict upon lysis of a mix population of cells by coliphage in the presence of substrate, the gene products will complement in trans reconstituting the beta-galactosidase activity thus eliminating a separation step in the assay. In addition we are testing the introduction of a cassette of coliphage cell lysis genes on both plasmids under the control of a coliphage promoter to accelerate the enzyme fragment release thus further reducing test time. As an alternative to the enzymatic read-out we are also exploring a nanoelectronic/microfluidic system to detect the phage-induced lysis of the target cells. Our goal is to design a fast-acting hand-held coliphage biosensor device that can be used by someone without any special technical expertise. We anticipate our device being useful in rapidly reporting the contamination of recreational waters in the U.S. or assuring potable water in the water sources in the developing World.
A number of theories argue that childhood experiences help shape adult personality, attitudes, and psychological functioning (Cassidy & Shaver, 1999). Adults who experienced more positive childhoods tend to function more positively than those who experienced overly negative parenting or abuse (Ruffo, 2007). Most research, however, has focused on the importance of the mother and has largely ignored the role of the father. The goal of the current study was to better understand connections between adult’s (current mothers’ and fathers’) caregiving history with their own mothers and fathers and the degree of parenting stress they currently experience with their own child. From an ongoing-study, data from twenty-two participants were used in the present study. The sample consisted of mothers and fathers who were married and cohabitating with an infant between the ages of 5 - 7 months. Mothers and fathers each completed questionnaires used to gauge stress (Parental Stress Index; Abidin, 1997) and caregiving history with their own mothers and fathers (Measure of Parenting Style; Parker et al., 1997). Correlational results indicated that mothers who experienced more abuse, over-control, and negative parenting by parents displayed a higher level of stress with their children. Contrastingly, fathers who had experienced more abuse, over-control and negative parenting by parents were less likely to view their children as difficult and reported an overall lower parenting stress score. These preliminary results underscore the importance of examining patterns for both mothers and fathers because processes connecting childhood experience and current parenting issues appear to differ.
In the current microelectronic industry power dissipation and the associated heat produced by devices represents a major problem. Modern microprocessors dissipate energy as heat, and this heat already limits their speed and packing density. However, studies have shown that more efficient devices are possible by changing the traditional computation method to one with lower energy dissipation. This research presents a novel approach for an energy efficient microprocessor. While current microprocessors use standard CMOS devices and computation technologies, the proposed design uses adiabatic computation to recycle energy. This new computation method uses ramping clocks to power the integrated circuit. These power clocks have adiabatic, or slow relative to RC time constants, changes between three different states. Charging and discharging the transistors in an adiabatic way, combined with reversible logic can avoid the dissipation of energy, since dissipation is only necessary when information is erased. This creates a more efficient microprocessor that dissipates much less energy than current devices. It should be noted that adiabatic clocking is only slow relative to the maximum transistor speed. Microprocessors already operate at frequencies well below the maximum due to power constraints. The final design consists of a complete semiconductor layout for an 8-bit MIPS microprocessor using adiabatic power clocks. The microarchitecture implemented is a multicycle non-pipeline RISC processor which supports a set of 10 different instructions. The entire microprocessor design is compatible with a standard CMOS fabrication process, therefore it will be fabricated using two different technologies: the Notre Dame 1.5um process, and the Mosis 0.5um C5 process. The design represents the first microprocessor of its kind.
Poster Presentation

Supporting critical care teams with shared interactive displays

Vanice Cheung
Michael Gonzales

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Medical errors contribute to an overwhelming number of deaths in the United States. Estimates go as far as saying that it is the third leading cause of death after heart disease and cancer (440,000 deaths per year) [1]. Not only is patient safety threatened, but there are also heavy financial repercussions, with estimated costs of over $1 billion in the United States in 2009 [2]. Our research goal is to use technology to improve response and reduce errors that result from poor team communication and low situational awareness. To do this, we aim to augment critical care procedures such as Pediatric Advanced Life Support (PALS) [3] and Advanced Cardiovascular Life Support (ACLS) [4] so that clinicians can be more cognizant while treating patients.

We first wanted to understand the structure of medical settings, including formal hospital procedures and informal hospital culture. We conducted qualitative ethnographic research through contextual inquiries and semi-structured interviews since recognizing the organizational system was critical as mistakes are often direct reflections of organization. We also collected relevant artifacts and documented room sizes and their layouts. Three hospitals were chosen as study cases - two midwestern regional hospitals (one a children’s hospital), and a regional hospital on the east coast. We transcribed and analyzed the collected data using content analysis by two independent coders. We calculated inter-rater reliability on a subset of our data (k-alpha = 0.79).

Our results suggest several critical design paths influenced by various factors. For example, environmental constraints, including space, movement, and positioning, vary from hospital to hospital. In addition, responses may be adjusted based on the type of patient (e.g. child vs. adult) and situation (simulation vs. real life). Conclusively, our findings underscored the importance of a clinician’s ability to modify an interface according to their specific response team and environment. Moving forward, we intend to use our findings in the design of shared user interfaces that could be used by multi-disciplinary code teams. In addition, we are developing tools that will allow physicians to construct their own algorithms to better suit their teams and environment.

Multipass optical cavities are widely used for applications in optical sensing because long path lengths increase the detection sensitivity of the systems. The most commonly used multipass cells are based on integrable dynamics using paraxial ray approximations, where integrability means that analytic descriptions of the ray dynamics can be specified. However, these optical systems have two major limitations: they consist of multiple focusing elements, which make their alignment nontrivial, and they must be of considerable length on the order of tens of centimeters for the ray dynamics to follow the paraxial ray approximations. To bypass these constraints, an optical cavity consisting of a single closed surface with quasichaotic ray dynamics was proposed. Here, we analyze the nonlinear ray dynamics of a quadrupole-shaped cavity and engineer the deformation parameters to obtain optical paths with greater length, stability, and global focusing. We model the optical beam as a point particle in a quadrupole-shaped cavity following the geometrical optics approximation and interpret the trajectory using the nonlinear classical dynamics formalism. We demonstrate that the stability of the transversal modes can be modeled as a simple function of the deformation variables, which makes it possible to find optimal quadrupole shapes for sensing applications.
Oral Presentation

Investigation into Anisotropic Nature of Ferromagnetic Resonance In Fe-GaMnAs

Devon Courtwright
Advisors: Jacek Furdyna, and Taehee Yoo, Dept. of Physics, University of Notre Dame

In this research we investigate the magnetic properties of a metal/semiconductor layered material grown by Molecular Beam Epitaxy (MBE). A Ferromagnetic Resonance Machine (FMR) is used to study what magnetic field strength is required to allow the sample to absorb incoming microwave radiation. Our specimen sample is a thin film of Fe grown on GaMnAs, with measurements taken at room temperature. The resonance peaks are demonstrated to have an angular dependence, while the emergence of multiple peaks are dependent on the direction of the applied field. Analysis of these peaks allows us to determine the anisotropic nature of the sample.
Tuberculosis (TB) is the second largest killer after HIV/AIDS among single infectious agents. Multi-drug resistant TB has been observed worldwide (WHO, 2014). The current vaccine for TB, the BCG vaccine, is not fully preventative and is not used in the US (CDC, 2014). To build a better vaccine, we need to expand our understanding of how the causative agent of TB, *Mycobacterium tuberculosis*, interacts with its host. *M. tuberculosis* requires an intact ESX-1 secretion system for virulence. The mechanism of how ESX-1 mediates virulence is unclear. We propose to identify novel genes required for ESX-1 secretion to clarify the mechanism of secretion. Our study used *Mycobacterium marinum*, an established model organism in which ESX-1 secretion is conserved and necessary for cytotoxicity to *Acanthamoeba castellanii*, a free-living phagocyte. To find unknown ESX-1 genetic components, we performed a screen on a transposon insertion library of *M. marinum* strains by testing their ability to lyse *A. castellanii*. We infected *A. castellanii* in 96 well plates with *M. marinum* strains at an unknown multiplicity of infection (MOI). We then selected for non-cytotoxic strains using optic microscopy. Non-cytotoxic strains underwent a second round of screening at an MOI of 10. Infection at MOI 10 was repeated twice for each strain. Strains that were non-cytotoxic in the second round of screening were further characterized by red blood cell lysis assay. Nine plates or ~750 strains were screened, and six mutant strains were identified. These strains also failed to lyse red blood cells, a mycobacterial phenotype that requires a functional ESX-1 system. Further characterization of the ESX-1 phenotypes as well as genetic mapping to determine the gene responsible for the phenotype are underway. Our study provides a screening method for ESX-1 deficient mycobacterial strains. These strains will be further studied to identify genetic components of ESX-1 secretion, thus enhancing our understanding of mycobacterial infection so it can be targeted and prevented.
Malaria is a mosquito-borne disease that affects millions of people each year, with over 600,000 deaths globally in 2012. Recently, Solomon Islands set a goal of nationwide malaria elimination. Decades of long-lasting insecticidal nets (LLIN) and indoor residual spraying (IRS) interventions have greatly reduced, but not eliminated malaria in Solomon Islands. Instead, the primary malaria vector, Anopheles farauti, has undergone a shift from late-night endophagic bloodfeeding to early-evening exophagic bloodfeeding. Presumably, these behaviors are selected for by LLINs and IRS, which may have reached the limit of their effectiveness. Thus, behavioral resistance could be a contributing factor to the persistence of malaria transmission. Our project will test the effectiveness of a novel outdoor intervention, insecticide-impregnated barriers (IIBs), at reducing malaria transmission over a period of 2 years. We conducted a baseline survey of malaria prevalence using 3,837 volunteer individuals in 19 villages across 5 islands in Western Province, Solomon Islands. The PCR-based survey revealed an overall malaria prevalence of 16.59%, with Plasmodium vivax accounting for the majority of infections. We also report here the first known occurrence of P. ovale in the Solomon Islands. This summer, we mapped study villages using geographic information system (GIS) devices, constructed IIBs in intervention villages, and distributed radical cure treatment to members of our incidence-monitoring cohort. The incidence of malaria infection in the cohorts will now be monitored over the next 2 years and compared between IIB villages and control villages with no intervention. Mosquitoes will also be collected in human landing catches to determine infection rates and changes in age structure over the ensuing study period. We hypothesize that the IIBs will reduce malaria transmission to almost zero over the study period as a result of the strategic placement of the interventions. We also hypothesize that the IIBs will target all mosquitoes increasing the daily mortality resulting in a shift to a younger age structure in the vector population.
Poster Presentation

*Biocomplexity and uncertainty: Science, technology, and ethics in the real-world case of silver nanoparticles in heavy commercial use*

Joshua Dempsey  
Kathleen Eggleson  
Advisor: Kathleen Eggleson, College of Engineering, University of Notre Dame

When it comes to the interface between emerging nanotechnologies and society, scientists and engineers are involved in complex ethical dilemmas and the challenge of just decision-making in the face of complexity and uncertainty. The aim of this undergraduate research project is the creative development of materials for the ethics education of graduate-level scientists and engineers on the macro (societal) level. Specifically, a hypothetical case-study has been developed for active learning with role play, a pedagogical approach demonstrated to enhance critical thinking and problem-solving skills in real-world situations. In the fictional scenario developed, students are given different roles to play as citizens and CEOs alike, and are presented with multiple ethical dilemmas spanning education of the public, risk assessment, precautionary principles, stakeholder theory, life cycle analysis, cost-benefit analysis, occupational health hazards, and stewardship of science. With the developed materials, students will gain a comprehensive understanding of the perspectives informing emerging technologies and societal decision-making, including historical examples such as the inclusion of radium in consumer products before potential health risks and occupational safety hazards had been adequately investigated and considered. Nanosilver is an emerging technology which parallels the story of radium to a degree. Antimicrobial consumer products containing nanosilver particles can be found online and on shelves at supermarkets, despite the fact that there is limited data on its cytotoxicity and a dearth of literature on its long-term environmental impacts.
DNA origami consists of single-strand viral DNA and short oligonucleotide staple strands, which self-assemble into nanoscale shapes and adhere to solid surfaces. It is known that DNA origami are more thermally stable when adhered to a solid mica surface than when in solution, but the temperature limits of this stability, and the effects of heating in different environments, were previously unknown. This thermal stability is potentially useful for lithographic applications and nanoelectronics, since many such processes require high temperatures.

DNA origami on mica were heated to temperatures up to 500°C in oxidative and inert environments, using a tube furnace that can heat the samples either in air or nitrogen. The nanostructures were then imaged using Atomic Force Microscopy (AFM) and the chemical characteristics of the surface were analyzed using X-ray Photoelectron Spectroscopy (XPS). Heating in a nitrogen-only environment greatly reduces thermal damage to DNA nanostructures. The DNA origami in both nitrogen and air maintain their areas as they are heated, up to the point where holes form in the origami. For the DNA in air, there were holes at 500°C, but the DNA in nitrogen remained intact even at 500°C. The height of the DNA nanostructures decreases with increasing temperature, up to the point where holes form. Once the DNA are sufficiently oxidized to form holes, there is an apparent increase in height as the DNA forms ridges around the holes. Nevertheless, even after heating at 500°C in air, the shapes of the origami are clearly visible.

Additional experiments could determine the amount of chemical degradation to the DNA after heating in nitrogen and air, and whether the DNA is damaged to the point that it can no longer base pair. Heating in a nitrogen-only environment should prevent the DNA from oxidizing, but there may be other chemical changes to the DNA. The results of this chemical analysis would determine the most appropriate potential applications, such as lithography, carbon nanotube growth, or burn-in doping for electronics.
Chemical genetic screening is the phenotypic assessment of small molecules to determine if they can alter signaling pathways affecting development, organogenesis, and/or other biological processes \textit{in vivo}. Zebrafish are a valuable model for chemical genetics due to their high degree of genetic conservation with humans and because their embryos can be easily drug treated by the addition of small molecules to the embryo media. It was previously found that retinoic acid (RA) signaling during zebrafish development is essential for renal progenitor patterning into discrete proximo-distal nephron cell type lineages from the intermediate mesoderm. It was also found that upon addition of exogenous RA, proximal segments expand at the cost of distal fates; conversely, inhibition of RA production using diethylaminobenzaldehyde (DEAB) eliminates proximal segment formation and expands the distal segments. Retinoic acid receptor alpha (RAR\textalpha) agonist AM-580 was shown to have similar effects as RA to promote proximal fates, while the RAR\textalpha antagonist R0 41-5232 inhibited proximal fates and expanded distal fates, suggesting a role for RAR\textalpha during renal progenitor development. However, further analysis of RA receptors during nephrogenesis has not been performed, hence we performed a chemical genetic screen using the ICCB Known Bioactives Library to gain novel insights into how RA and other molecules affect nephrogenesis. We found that 78/480 compounds induced morphological defects in the pronephros. Among them are compounds that regulate peroxisome proliferator-activated receptor (PPAR) activity, thus suggesting a previously uncharacterized role for PPARs in addition to RAR\textalpha for proper renal development. We selected this pathway for in-depth characterization and have further shown that PPAR\alpha agonist bezafibrate works to promote proximal segments at the expense of distal segments in a fashion similar to exogenous RA treatments. Future studies will delineate the time window when alterations in PPAR activity affect nephrogenesis and identify the specific genes that are involved. As PPAR coregulators have been used in the treatment of diabetic nephropathy, understanding how they affect development is critical, and this research has translational value because this drug’s effect on establishing segmentation boundaries in the kidney may ameliorate renal progenitor mispatterning in humans.
Poster Presentation

*Using the Natural Bond Orbitals of Ionic Liquids to Predict Relative CO₂ Binding Strength*

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Ionic liquids can bind selectively and reversibly with CO₂. This allows ionic liquids to be an effective and environmentally friendly way to reduce CO₂ emissions. The important chemical properties of ionic liquids that allow for CO₂ capture are caused by its electronic structure. The goal of this research is to better understand the electronic structure of ionic liquids, in order to predict the relative strength of CO₂ capture. To do this, Natural Bond Orbital analysis is used. NBO analysis is an effective computational method which can represent a complicated electronic structure as “Lewis-like” orbitals. This allows for a localized understanding of charge and energy. This research uses the NBO analysis on a one ion pair module of several different ionic liquids, in order to determine the effects that orbital energy and charge have on CO₂ binding. While it was previously reported that an anion only module was unable to predict relative CO₂ binding enthalpy, the ion pair module is able to predict the relative CO₂ binding enthalpy. It was found that the anion’s orbital energy and charge depended on the cation, as well as the distance between the cation and anion, further showing the importance of the cation’s role in CO₂ binding. The orbital energy and charge of the CO₂ reaction site were found to be linearly related to the CO₂ binding enthalpy.
This research explores the ability of plasma treatment to prevent toxic plasticizers from leaching from PVC products. In this research, Fourier transform infrared spectroscopy (FTIR) was used to investigate the bulk structural changes of plasticized poly(vinyl chloride) (PVC) due to microwave exposure at a molecular level. PVC containing 25 wt% Bis-2-ethyl-hexyl phthalate (DEHP) plasticizer and pure PVC films were exposed to microwaves for a three-minute period with 2000 µl of deionized water and IR spectra were obtained before and after to study plasticizer leaching. To study the viability of plasma treatment for leaching prevention, etc., select films were exposed to either air or argon plasma treatment for 5 seconds prior to microwaving. In argon plasma treated films, more DEHP remained in the plastic after microwaving compared to the non-treated films whereas air plasma treated films experienced greater DEHP loss than non-treated films. From this data, it can be shown that argon plasma creates a minor shielding effect to prevent some plasticizer leaching from bulk while air plasma promotes plasticizer loss When exposed to microwaves multiple times, plasticized films continue to demonstrate leaching so any protective effects from plasma treatment are lost. Microwaves promote plasticizer leaching, and plasma treatment is not a valid method to prevent this leaching.
Oral Presentation

*Dynamic Provisioning of Custom Clusters Through HTCondor and Openstack*

Stephen Ennis
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The rise of Cloud IaaS (Infrastructure as a Service) presents many opportunities for the scientific community to make increasingly efficient and effective use of local and external distributed resources. This paper examines how some aspects of job and cloud management may be combined. In particular, we examine the possibility of joining job submission with the creation of dynamic cloud resources to mimic idealized opportunistic grid computing. During this project we made use of the private OpenStack IaaS cloud facilities and HTCondor grid scheduling engine managed by the Center for Research Computing at the University of Notre Dame Indiana. In this work we provide information regarding the combination HTCondor and OpenStack facilities to improve ease of use and QoS for end users in science. A sample application utilizing a biochemistry based workflow is provided. We examine the challenges, drawbacks and benefits relating to the dynamic (on-demand) creation of custom clusters on shared cloud resources for the completion of scientific workflows.
Carbon sp3-halogen bonds are important in pharmaceuticals, agrochemicals, and natural product syntheses and generally serve as ideal coupling partners in numerous important transformations. While these functionalities are difficult to form through traditional Pd0/PdII catalysis, recently PdII/PdIV catalytic systems have been shown to be useful in constructing these bonds. Despite their importance, detailed studies investigating the mechanism of proposed PdIV intermediates are limited. Therefore, a mechanistic exploration would allow for greater understanding of carbon-halogen bond forming reductive elimination at PdIV centers, which would lead to greater understanding and improvements in rate and selectivity of palladium catalyzed reactions. We report competing sp3-C-X (X = Cl, Br, I) and sp3-C-F bond forming reductive elimination at PdIV centers and the factors that lead to different selectivities. A variety of experiments, including Eyring plots, crossover studies, ligand effects, halogen effects and solvent effects provide preliminary insight into the rate and mechanism of sp3-C-halogen reductive elimination.
It has been estimated that more than 10% of all electricity is lost during power conversion. This lost happens when electricity is converted from one voltage to another, from AC to DC, or from DC to AC. Transistors made from GaN are being investigated for more efficient high-power applications that can switch 100 A with a maximum operating voltage of 1,200V. This project used Synopsys Sentaurus TCAD to evaluate the performance of different GaN vertical junction field-effect transistors based on device dimensions and doping levels. In addition an energy curriculum was also produced to teach at the 7th grade level.
A complex problem in lower income regions of the world is the abundance of sub-standard pharmaceuticals. About 25% – 30% of the pharmaceuticals from Kenya tested to contain sub-standard or no Active Pharmaceutical Ingredients (APIs) – low quality or counterfeit medications. The traditional technique used for drug analysis involves the use of expensive equipment such as a High-Performance Liquid Chromatography (HPLC), or a Mass Spectrometer. We are developing a low cost technique using paper technology to perform the analysis of the drugs. We are doing this by developing “lane tests” which test for a specific API in a pharmaceutical. I found that we could use turmeric as a test for borate/boric acid and as a pH indicator, and sodium nitroprusside in combination with potassium ferricyanide and sodium hydroxide to test for an API in Streptomycin and other similar pharmaceuticals. To analyze a drug, we spot the Paper Analytical Device (PAD) with twelve lane tests and run it with a single drug. Then we use an image analysis program to analyze the result from the PAD test. Twenty six pharmaceuticals and excipients including water, as control, had to be tested in three dose levels (light, medium and heavy dosages), on sixteen different tests resulting in four-hundred and sixteen tests in order to create a database of test outcomes for the image analysis program. This collection of data in the database is going to serve as reference for the PAD analysis program, which will use the reference data in the database to make a decision and provide feedback to the user on the authenticity of the sample. Figure 1 below shows a full PAD test on Isoniazid-Starch sample mixture.
Oral Presentation

*Modernizing Plunger Control with Low-Cost Digital Electronics*

Patrick Fasano  
Trenton Kuta  
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The plunger technique provides a valuable tool for measuring lifetimes of excited states in the 1-100 ps range. The plunger consists of a thin foil target and stopper foil separated by some controllable distance; beam-induced reactions occur in the target and the resulting nucleus of interest leaves the target foil and is completely stopped by the stopper foil. The Doppler-shift in $\gamma$-ray energy due to the velocity of the de-exiting recoiling nucleus is used to count the fraction of transitions which occur during the flight time, thus giving the mean lifetime of the gamma-ray depopulating a specific nuclear state directly. This technique, called the Recoil Distance Doppler-Shift (RDDS) method, requires precise and stable positioning of the foils over periods of hours or longer while correcting for beam-induced deformations to the foils.

The Notre Dame Nuclear Science Laboratory has a plunger device which is approximately 30 years old. Our work this summer included the upgrade and full rebuilding of the electronics to control the plunger system. In the Notre Dame plunger apparatus, the separation between foils is measured via capacitance between the foils and is used to control the position of three servo motors. We have made two major upgrades to the plunger device: (1) a newly-applied, precision capacitance-measuring circuit based on the phase-shift of a sinusoidal signal, (2) and low-cost microcontroller-based feedback loop for precisely controlling servo motors with quadrature encoder outputs. The capacitance measurement follows a development in the mid 1990’s that will now be applied to the ND plunger. The microcontrollers are also a significant modernization of the plunger. Once we have demonstrated that all the mechanical parts of the plunger work as desired, we will carry out reactions in the Nuclear Science Laboratory and will measure the lifetimes of excited states in several rare earth nuclei.
The World Health Organization (WHO) published the WHO Roadmap in 2011 as a plan to eliminate 17 neglected tropical diseases, such as lymphatic filariasis, by the year 2020. WHO’s recommended strategy of mass drug administration is an annual treatment of two medicines, ivermectin plus albendazole or DEC (diethylcarbamizine) plus albendazole, depending on whether the area is co-endemic or not, respectfully. Other intervention methods like use of bed nets or light traps are also tools for disease control. Mathematical models allow for a quantitative way in analyzing methods to control and eliminate diseases. Modeling lends insight on the current status of disease eradication and how far progress has been made in terms of eliminating the disease. These models provide information on the effects of measures used to control disease, for example, use of mass drug administrations or other intervention methods. In order to make these models accessible to the larger scientific community, a portal, in such settings also called science gateway, is desired. Science gateways bundle various tools and applications to be accessed in an intuitive way. These science gateways provide easy access to computational resources as well as data, and capabilities like data management or job execution services. This science gateway is built with the Agave (a grid and virtualization environment) API, which has many features built in, like system management, an application catalog, job execution, data and metadata management, and notifications. Web development technologies including HTML5, CSS, JQuery, and Ajax were used to construct the portal. Currently, the portal supports job execution, application selection, file input selection, and job polling. Future work includes functionalities to browse and download job output on the portal, using cloud resources, and implementing different views for different kinds of users.
Poster Presentation

Auto-prober I-V Measurements – How To Measure 100 Devices In 60 Minutes

Patrick Foley
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Traditional probe stations require the manual movement and placement of probes on a device in order to measure the device characteristics. The Cascade Summit 12000B-M is installed with Nucleus, which is a software used for automated movements. Nucleus can be used with DC characterization applications, such as Wavevue, to automate the testing of hundreds of devices. Wavevue is an integrated measurement solution that unifies RF/microwave and DC measurements in one software application. The Wavevue software can do many useful measurements, and automatically builds reports for the user once the measurements have finished. The goal of the project was to utilize the software to test many devices, accumulating results quickly and efficiently for samples fabricated by graduate students. The process of using the two software programs in unison was detailed and used to measure current-voltage characteristics and breakdown voltage of metal oxide silicon heterostructures.
Poster Presentation

The Iterative Second-Order Green’s Function Method (GF2) for Electron Correlation

Brad Ganoe
Jordan J. Phillips
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The development of computationally feasible and generally accessible many-body methods, which are indispensible towards the description of electronic correlation, is a necessity for accurate quantum chemical calculations. We develop an ab initio iterative Green’s function method using an implicit resummation of Feynman diagrams up to second-order (GF2). Self-consistency is achieved through an iterative solution of the Dyson equation, with an imaginary frequency domain Green’s function and imaginary time domain self-energy. The implementation allows for a single-reference formalism that remains black box capable and computationally tractable. The GF2 method is applied to prototypical examples, such as He dimer and H12, to determine its effectiveness for molecular systems. Results indicate that iterative Green’s function methods are an attractive alternative to traditional many-body theory due to its accuracy, low computational scaling, and description of some strong correlation effects.
Inhibition of MMP-12 and ADAM10 by DR-04-086

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Derong Ding
Jamarcus Payton
Advisors: Shahriar Mobashery and Mayland Chang, Dept. of Chemistry and Biochemistry, University of Notre Dame

A Disintegrin and metalloproteinase domain-containing protein 10 (ADAM10) has been shown to have α-secretase activity with amyloid precursor protein (APP) as the substrate. Selective inhibition of ADAM10 can be useful in elucidation of the biological role of this enzyme in neurological ailments. DR-4-86 has been reported as a selective inhibitor of ADAM10 (Cancer Biology & Therapy 2006, 5, 657-664). This compound was synthesized in our lab and its profile in inhibition of a series of ADAMs and the related matrix metalloproteinases (MMPs) was investigated. The presenter, JaMarcus Payton, addressed analysis of inhibition of DR-4-86 by a method other than what was analyzed in the lab earlier. The Lineweaver-Burk plot as an alternative method to the Dixon analysis indicated that ADAM10 and MMP-12 were inhibited potently with patterns of inhibitions that were linear noncompetitive with dissociation constant of 85.5 ± 10.4 nM for ADAM10 and 223 ± 18 nM for MMP-12.
Poster Presentation

A quantitative estimation of trap stiffness using a CMOS camera

John Gensic
Zhongming Li
Mary Sajini Devadas
Matthew Bartels
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Lasers are used to build optical traps to study the physics behind the manipulation of nanoparticles. These optical traps were first used in the 1970s and have many applications for single particle studies in cell biology as well as physical chemistry. Because it can capture not only individual cells, latex beads, but also noble metal nanoparticles, it enables us to obtain accurate and in-depth information of single particles. Trap stiffness is an important index of optical trapping, because it basically defines how stable and stiff the trap is, despite the effects of Brownian motion and thermal noise. In this study, the influence of size of the particles, power of the trapping laser, effect of polarization of the laser and camera speed on trap stiffness were studied.
The St. ANA (STable Accelerator for Nuclear Astrophysics) accelerator is being prepared for use with the St. George recoil mass separator. The accelerator is in working condition for use in direct kinematic experiments but the St. George separator works with inverse kinematics and requires a highly controlled beam restricted by severe position and divergence parameters that are not achieved at the present time. A systematic sensitivity study was conducted using a simulation of the beam line in order to assess the impact of a misalignment in each optical element or in the beam itself. Tests were done with the beam to analyze how the beam behaves at various points in the line and to compare this data with simulation results to determine possible causes of misalignment. The results of these tests and simulations are that the beam characteristics are now better understood and the possible causes of the limitations have been narrowed down.
Mosquito-borne diseases represent an immense global health burden, afflicting hundreds of millions of people worldwide. Insecticides have always been one of the most effective forms of combatting the transmission of these diseases. However, widespread insecticide resistance poses a major challenge to vector control initiatives, necessitating the development of novel insecticides. The membrane bound signaling molecules, G protein-coupled receptors (GPCRs) are promising candidates for insecticide development. These receptors are involved in many indispensable physiological processes in insects, and appear to act as neuromodulators of olfaction, locomotion, and development. This study focuses on the tachykinin receptor of *Anopheles gambiae*. Using real time PCR, the expression of the receptor was quantified in all life stages of the mosquito. Using, molecular cloning, the tachykinin receptor was cloned into a luciferase reporter construct and transfected into HEK-293 cells. Furthermore, the ligands for the receptor were predicted using comparative genomics. The establishment of a stable cell line and the prediction of the receptor ligands will allow future research to test potentially insecticidal compounds against the tachykinin receptor.
Increasing evidence supports the concept that instances of cancer recurrence may be due to a subpopulation of cells within a tumor that behave like stem cells. Previous studies have demonstrated that pathways critical in oncogenesis parallel those necessary for the induction of pluripotency, suggesting that similar mechanisms regulate both processes. By therefore understanding the mechanisms that govern reprogramming, we may gain insight into the methods by which cancer cells acquire and exploit stem cell properties, and enable more strategic targeting of these cell populations to prevent malignant relapse. Glucose-regulated protein 78 (GRP78) is a molecular chaperone protein that is generally restricted to the endoplasmic reticulum in normal tissues, but is aberrantly expressed at the cell surface in many types of tumors. Furthermore, targeting GRP78 in mouse models suppresses tumor growth, and cell surface GRP78 has been shown to be a molecular target on human tumor samples. Although these studies have suggested an important role for GRP78 in promoting tumorigenesis, the mechanisms are not yet fully understood. We have previously shown that GRP78 plays an important role in somatic cell reprogramming, or the ability of an adult cell to acquire a pluripotent state. To next examine the function of GRP78 in stem cell regulation and determine the ability of GRP78 to contribute to a stem-like phenotype in cancer cells, we have developed a breast cancer cell line (MDA-MB-231) that expresses RFP-GRP78 under a doxycycline-inducible promoter. We have found that overexpressing GRP78 in MDA-MB-231 cells induces the expression of genes normally only expressed in pluripotent stem cells. Given our previous findings that GRP78 plays an important role in the reprogramming process, and the known function of GRP78 in tumorigenesis, these data suggest that GRP78 may contribute to the generation of a stem-like response in cancer cells. To expand on our findings and better understand the role of GRP78 in pluripotent stem cells, we have reprogrammed the MDA-MB-231 cell line containing inducible RFP-GRP78. Expansion and characterization of individual iPSC clonal lines are ongoing. These iPSC lines will provide a valuable tool to study the function of GRP78 in human pluripotent stem cells.
Oral Presentation

**ARID3B regulates stem cell adhesion through CD133**

Karolina Gogola  
Alexander Bobbs  
Advisor: Karen Cowden Dahl, Dept. of Chemistry and Biochemistry, University of Notre Dame

Ovarian cancer is the fifth leading cancer death in women because of its high incidence of metastasis and recurrence. Our lab studies the DNA binding protein ARID3B that plays a role in development yet is over expressed in ovarian cancer. Little is known about ARID3B, but a mouse model completed by our lab has surfaced new information. Mice injected with SKOV3IP ovarian cancer cells that over express ARID3B grew tumors that were more than 2.5X larger than SKOV3IP-RFP (red fluorescent protein) (control) cells that were injected into mice. Analysis of the SKOV3IP, SKOV3IP-RFP, and SKOV3IP-ARID3B through flow cytometry showed an increase in cells expressing CD133, a cancer stem cell marker, in the SKOV3IP-ARID3B cells compared to controls. Also, quantitative reverse transcribed polymerase chain reaction (QRT-PCR) revealed increased CD133 mRNA expression in SKOV3IP-ARID3B cells compared to SKOV3IP-RFP cells. Therefore, our lab’s research shows that ARID3B increases cancer stem cell production. Currently, we are further researching the stem cell marker CD133 because very little is known about CD133’s function. We hypothesize that ARID3B transcriptionally regulates CD133 and that CD133 increases cell adhesion. We have been able to show that the presence of CD133 through transfection of OVCA429 cells produces hair-like membrane protrusions. We hypothesize that CD133 uses these protrusions to increase cell-cell adhesion, especially to mesothelial cells. When comparing cells transfected with CD133-GFP (green fluorescent protein) to cells transfected with only GFP, the GFP cells did not show the hair-like structures observed in the CD133 cells. Although an ECM assay showed no considerable difference in adhesion between transfected CD133 cells and control cells, we are repeating transfections to obtain a better yield of the number of cells that are transfected with the PROM1 (CD133) DNA in order to repeat adhesion assays. Currently, we are furthering our research by using siRNA to knockdown CD133 in cell lines SKOV3IP, SKOV3IP-RFP, and SKOV3IP-ARID3BFL to determine if CD133 affects adhesion. This study will demonstrate ARID3B regulation of CD133 and the role of CD133 in adhesion.
Blastocystis spp. is a protozoan intestinal parasite that belongs to the Stramenopile group. Little is known about its virulence. It seems to have low host specificity and virulence varies even within the same host species. In some studies, a certain subtype may show virulence within a host, but in other studies it shows no virulence. It has been suggested that there may be genetic factors that differ between the different subtypes of the parasite, of which there are 13, that may be the cause for this variation in virulence expression. This study was focused on designing primers for virulence factors, which have been annotated in the Blastocystis genome. By looking at patterns of genetic variation associated with virulence factors, we can begin to understand how virulence may be controlled in this pathogen. To design primers, several steps were taken. First, all possible virulence factor candidate proteins were identified and listed. The criteria used to select the proteins were: direct or indirect interaction with immune system molecules, capacity to inflict tissue damage and/or proteins that were homologs of known virulence factors. Second, the list was refined to narrow it down to the most probable candidates. Once the list was screened and narrowed down, the sequence for each locus was searched to design appropriate primers for amplification of virulence factors. We chose 13 loci to analyze, six of which we designed primers for our tests. These include gamma interferon inducible lysosomal thiol reductase and immunoglobulin heavy chain binding loci. With this study, the virulence factors of Blastocystis have been identified and primers have been created for them. In the future, this study will enable a more thorough analysis of these factors, which may shed light on the difference in virulence between subtypes.
Nitrous oxide (N2O) is an important greenhouse gas with a global warming potential 300 times greater than carbon dioxide (CO2). Biological wastewater treatment, which uses nitrification and denitrification, has been shown to be a significant anthropogenic source of N2O. Dissolved oxygen (D.O.) is an important factor leading to N2O formation in conventional, suspended-growth wastewater systems. However, little is known about the effects of D.O. on N2O formation in biofilm-based treatment processes, which are increasingly popular. This study evaluates the effect of D.O. on the production of N2O in biofilm systems. Two different systems were used: a Moving Bed Biofilm Reactor and a fixed bed reactor. The reactors were used to develop nitrifying and denitrifying biofilms, respectively. The nitrifying biofilm was very thin, while the denitrifying biofilm was much thicker.

Results showed that the maximum rates of N2O production from nitrifying biofilm occurred at 0.3-0.7 mg/L. In the denitrifying process, the maximum production of N2O occurred at a D.O. of 1 mg/L. The D.O. concentration highly impacted the N2O in both processes, with lower N2O emissions at very high and low value of D.O. Past research shows that N2O formation in suspended growth systems is maximal at 1 mg/L D.O. for nitrification and 0.3 mg/L D.O. for denitrification. The nitrification results were similar to suspended growth, which was expected as the biofilm was very thin. However, the maximum denitrification occurred at a much higher value than for suspended growth. This may have resulted from the D.O. gradients in the thick biofilm.

Our results suggest that biofilm processes behave differently from suspended growth systems, probably due to oxygen gradients within the biofilm. These differences should be studied in more detail to determine if biofilms systems may pose a greater concern for global warming.
Ionic liquids (ILs) have many properties that make them an attractive candidate for replacing organic solvents in ion-lithium batteries. ILs are highly conductive, have negligible vapor pressure and thermally stable to high temperatures. This work investigates the effect of water on the electrical conductivity of select ILs while monitoring the density and viscosity. ILs readily absorb water and will likely contain water in any practical application. For the ILs investigated, water had no impact on the conductivity up to 1 weight percent water. Additional water after 1 weight percent up to 10 weight percent water increased the conductivity as the viscosity dropped according to the expected trend described by the Walden rule. Additional water after 10 weight percent significantly dropped performance.
In recent years, parts of the United States have sustained damage to fresh fruit crops due to the presence of *Drosophila suzukii*, an invasive, pestiferous species of fruit fly that is unique in its ability to oviposit in and feed on fresh fruit. Traditional methods of population control have been ineffective because the baits are not species-specific, leading to the capture of many arthropod species, including other fruit flies. Thus, the main objective of this study is to identify baits that are optimal for *D. suzukii* attraction in order to improve monitoring traps. Olfaction plays a key role in *D. suzukii* behaviors, such as host attraction and oviposition, due to the presence of yeast volatiles on fruit substrates. Previous research on the association between *D. suzukii* and yeast used gas chromatography linked electroantennogram detection (GC-EAD) to identify the most biologically active chemical components of the yeast odor profiles. My project used electroantennography (EAG) to determine which concentrations of those compounds produce the greatest differential response between *D. suzukii* and *D. melanogaster*. Each compound was tested on males and females of both species at two different concentrations. Preliminary data shows that there are significant differences in electrophysiological response to four different compounds: butyl acetate, isoamyl acetate, isobutyl acetate and ethyl hexanoate. Specifically, *D. suzukii* had greater responses to butyl acetate, isoamyl acetate, and isobutyl acetate than *D. melanogaster* at both concentrations, while *D. melanogaster* had greater responses to ethyl hexanoate. These results imply that there are differences in compound sensitivity between these species, which means that these compounds could be used as species-specific baits.
Poster Presentation

*Electrodeposition of reduced graphene oxide on metal oxide substrates: effect of loading on activity in heterogeneous Co(S₂C₆H₂Cl₂H₂)₂ dihydrogen production systems*

Jordan Gregory  
Diamond Thomas  
Shawn Eady  
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For the development of sustainable dihydrogen production systems, heterogeneous catalysts manifolds are ideal for use in industrial application involving fuel cells and for use on semiconductor surfaces to provide direct solar energy to (chemical) fuel conservation. The electrostatic adsorption of catalysts onto graphitic surfaces via conjugated ligand moieties provides a facile and inexpensive means to afford heterogeneous catalyst systems. This method has been shown effective for several catalyst models, recently including cobalt bis(dithiolate) dihydrogen production catalysts adsorbed on reduced graphene oxide (RGO)-coated substrates. The heterogeneous manifolds afforded were shown to be very active, stable to aerobic atmosphere, and simple both to prepare and adsorb on the RGO surfaces. The focus of this research is to modify the fluorine-doped tin oxide (FTO) substrate surfaces by varying the loading of electrodeposited RGO, and to determine the effect on overall catalyst activity in the resulting heterogeneous catalyst systems. Cyclic voltammetry studies were performed to estimate the comparative amount of RGO deposited on each substrate, and for subsequent activity analysis of the catalyst-soaked surfaces in acid solution. The systematic analysis of RGO loading effects on catalyst activity studied here provides insight for the development of other heterogeneous manifolds using RGO interfaces. In addition, since RGO can be easily deposited onto a variety of substrates, the catalyst system studied here could be applied to semiconductors surfaces to provide sunlight-driven dihydrogen production systems using inexpensive and easily accessible materials.
Given the properties of diamond, synthesis methods that offer control over its morphology and composition while being rapid and cost-effective can be advantageous. One such method of production includes chemical vapor deposition enhanced via a direct current microplasma. Though μPECVD has been shown to produce nanodiamonds under certain conditions, the exact mechanisms of nanodiamond growth and deposition are not precisely understood. The sheer number of parameters involved in μPECVD requires careful consideration of the apparatus and conditions needed to grow nanodiamond nonetheless control its morphology and composition. The apparatus consists of a vacuum chamber, a high voltage power supply, a substrate heater, and mass flow controllers. These components enable regulation of pressure, plasma behavior, substrate temperature, and gas flux. To safely incorporate all components, the apparatus needs vacuum compatible thermal and electrical insulation. The conditions for μPECVD of nanodiamond have been determined through experimental investigation and literature searches. Conditions over which the plasma exhibits stable behavior have been documented visually through the use of videography and photography while all others have been obtained from cited values. In short, this work presents an apparatus and preliminary conditions appropriate for μPECVD of nanodiamond.
Oral Presentation

*Graphitization Method for Carbon-14 AMS Measurement*

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The Accelerator Mass Spectrometry (AMS) group at Notre Dame is currently working on implementing a reliable method to perform an AMS measurement of the Carbon-14 concentration in a sample. Carbon-14 is the most commonly measured element in AMS due its applications in many different areas of study including biology, archeology, environmental science and hydrology. There are two standard procedures for sample preparation. The procedure we need to perform depends on whether the ion source relies on solid or gas cathode material. Our summer project was focused on the development of a graphitization line. This line will enable our group to run carbon-14 samples in the accelerator by having a simple and brief process that converts a sample into graphite, which is essential for a reliable AMS measurement of Carbon-14.
Heterogeneous catalyst manifolds composed of non-precious metals for the production of dihydrogen are of great importance to sustainable energy research for ease of use in fuel cells and application in photocathode systems. Electrostatic adsorption of catalysts onto graphitic surfaces is a simple and inexpensive yet effective means of affording heterogeneous systems. A variety of catalysts containing conjugated ligand systems have been reported in literature to retain activity adsorbed on graphitic surfaces such as reduced graphene oxide (RGO). Cobaloximes are a class of bis(dimethylglyoximato)cobalt(III) complexes that are widely known to be active dihydrogen production catalysts in neutral pH solutions. Very little research has been done on cobaloximes in the heterogeneous phase, although initial studies suggest activity of cobaloxime derivatives is retained after surface attachment. This research focuses on synthesizing conjugated pyridine-based tethers for the electrostatic binding of cobaloximes to RGO surfaces. A systematic approach was taken to discover the effects on binding strength of each axial pyridine ligand by varying the size and electron density of the conjugated system that adsorbs to the RGO surface, as well as the alkyl chain length connecting the aromatic moiety and the ligated pyridine. Cyclic voltammetry (CV) experiments were used to assess the activity and stability of the bound cobaloxime species. As RGO can be easily deposited onto a variety of substrates, the catalyst system studied here could be applied to semiconductors surfaces to provide sunlight-driven dihydrogen production systems using inexpensive and easily accessible materials. Further, the systematic analysis of various conjugated ligands and the resulting electrostatic adsorption on RGO provides insight for the development of other heterogeneous manifolds using a graphitic interface.
Regulation of the all-important process of gene-expression is known to occur at a variety of levels and by a plethora of mechanisms; perhaps one of the more complex and therefore less understood mechanisms by which expression is controlled is that of splicing. During splicing, a group of functional RNAs and proteins collectively referred to as the “spliceosome” removes intronic RNA sequences from pre-messenger RNA (pre-mRNA), via two transesterification reactions per section (intron) removed, resulting in a nonstop coding region that can be translated into a specific protein. This process can also remove different combinations of exonic DNA sequences along a gene, resulting in the ability of one gene to create more than one protein. Splicing is therefore a key process in organisms with more intricate genomes, and ongoing problems with this process result in serious disease conditions for the whole. The formation and disassociation of the spliceosome along a pre-mRNA substrate involves a large number of proteins and RNAs that interact in subtle ways with each other and with each specific substrate. With RNA as both substrate and a large part of the enzymatic machinery, it is no surprise that helicases – or RNA unwinding machines – have been found to play a fundamental role in the dynamic function of the spliceosome. In the experiments described here, the activity of the DEAH-box spliceosomal helicase Prp22 was probed using smFRET technology and different RNA substrates. Bulk and smFRET activities were also compared to a well-studied viral helicase, NS3.
Gamma-ray bursts (GRBs) represent “the most powerful explosions in the universe since the big bang” and the nature and the origin of GRBs remain a mystery. Understanding these can help us understand the stellar evolution, how black hole works, etc. However, most detections of Gamma-ray burst are limited in the low energy range. For example, Swift (Swift Gamma-Ray Burst Mission) covers the energy range 0.3-150keV; Fermi (Fermi Gamma-ray Space Telescope) covers the energy range 10kev-300GeV. Project GRAND is an air-shower detector array which is sensitive to 30-300GeV and 100-100 000TeV energies. Using the data from GRAND, we analyzed some of the GRBs which were detected by the satellite mission. Specifically, we extracted GRAND data during the time when GRBs happened and tried to find the increase of muons number to decide if we had observed the GRBs within our energy range. Another line of research this summer concerned UW Coronae Borealis (UW CrB). UW CrB is a low-mass X-ray binary system with a neutron star primary. Here we present the photometry made from the CCD images taken by LBT (Large Binocular Telescope) on June 30th while it simultaneously obtained spectra. We found a flare in the photometry, which represents an X-ray burst event from fusion on the neutron star. We confirm the flare and two other possible flares in an analysis of VATT photometry taken the same night as the LBT data.
Poster Presentation

AS-PCR as a Diagnostic for Differentiating Between Anopheles funestus Chromosomal Forms: Folonzo and Kiribina

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Anopheles funestus is regarded as one of the most important African vectors of malaria. In Burkina Faso, researchers have identified two different chromosomal forms of this species—Folonzo and Kiribina, that inhabit the same geographic area. Despite their closeness, they do not seem to interbreed, as indicated by the lack of heterokaryotypes. These forms exhibit a difference in behavioral patterns that can affect the control and prevention of malaria transmission. Because current methods of distinguishing between these forms are difficult and costly, this study looks to investigate Allele Specific-PCR as a method for differentiation between Folonzo and Kiribina. Next generation sequencing of DNA samples from Kuiti was used to identify fixed single nucleotide polymorphisms (SNPs) between the two forms—which served as the targets for the design of nine site-specific primer cocktails. Each cocktail, containing forward and reverse primers for Folonzo and Kiribina, was tested on remaining Kuiti DNA. Of the nine cocktails, two were successful in accurately differentiating between the two chromosomal forms with 90% accuracy or better—including failed, abnormal, and incorrect results. When successful primers were tested on karyotyped specimens from neighboring villages, Bagre and Dirze, PCR products did not exhibit the expected banding patterns. These results indicate the presence of a fixed SNP in the Kuiti population that may not be present in the Bagre and Dirze populations, possibly due to geographical distance. Future research includes testing of additional samples from villages surrounding Kuiti, to assess the distribution of the targeted SNP and identifying other areas for fixed SNPs that might be distributed among all Folonzo and Kiribina populations.
Polycyclic heterocyclic scaffolds have a wide presence in pharmaceuticals and biologically active natural products. As such, efficient and versatile methods for their syntheses are important for the discovery of new drug leads. To this end, we report a novel tandem Pd-catalyzed carboamination/Diels-Alder [4+2] cycloaddition reaction that affords unprecedented polycyclic N-heterocyclic compounds in moderate to excellent yields with up to >20:1 diastereoselectivity. These reactions are beneficial as they can rapidly afford complex products from simple precursors. In order to expand the scope of this reaction, different substrates have been investigated. In this case, we focused on ethyl (E)-4-oxo-4-(pent-4-en-1-ylamino)but-2-enoate, which bears an electron deficient dienophile. By varying the reaction conditions, we determined viable reaction conditions that effect a Pd-catalyzed alkene difunctionalization reaction and subsequent Diels-Alder cyclization. The starting material was synthesized in three steps and then subjected to the catalytic reaction involving 9-bromoanthracene, Pd(OAc)$_2$, DPE-Phos, Cs$_2$CO$_3$, and dioxane. The tandem reaction proceeds in a one flask operation to afford the desired polycyclic pyrrolidine product with an isolated yield of 35.9% (60% average yield per step) and >20:1 dr. Three stereocenters and four bonds (3 C-C and 1 C-N) are generated over the course of the reaction. Investigations are currently underway for the new substrate to undergo a Diels-Alder cyclization. We hope the more electron deficient dienophiles will expand the scope of the allowable dienes.
The World Health Organization (WHO) estimates that over 39 million people worldwide suffer from blindness, with an additional 246 million suffering from other types of visual impairment. Zebrafish (*Danio rerio*) are a valuable degenerative/regenerative model system because unlike humans, zebrafish can regenerate lost retinal neurons in response to damage and ultimately restore vision. Upon damage to the zebrafish retina, Müller glia reenter the cell cycle, produce progenitors that continue to proliferate, migrate to the site of damage, and differentiate into the lost retinal cells (Vihtelic et al 2006). The mechanisms that induce Müller glia dedifferentiation to generate neuronal progenitors and the subsequent regeneration process are not fully characterized. Previously, our lab demonstrated that the undamaged retina expresses Pax6 in amacrine and retinal ganglion cells, but upon retinal damage, Pax6 is upregulated in columns of proliferative progenitor cells (Thummel, 2008). Quantitative PCR demonstrated that two Pax6 paralogs, pax6a and pax6b, are differentially regulated and morpholino-mediated gene knockdown indicates they possess different functions: Pax6b knockdown stops neuronal progenitor cells from undergoing the first progenitor cell division, while Pax6a knockdown prevents subsequent cell divisions (Thummel et al 2008). As a first step to determine the role of Pax6a and Pax6b in neuronal progenitor cell proliferation during zebrafish photoreceptor regeneration, I generated a transgenic line using transposon-mediated BAC transgenesis that expresses GFP from the pax6b promoter. Pax6b expression is localized to the brain, spinal cord, pancreas, and retina of the developing zebrafish embryo. Retinal cross sections demonstrate GFP-positive cells in the INL and GCL and immunohistochemistry confirmed that GFP expression is confined to neuronal progenitors, amacrine cells, and retinal ganglion cells in the transgenic line. A pax6b specific DIG-labeled anti-sense RNA probe was generated to validate the endogenous expression of pax6b in the transgenic line using in situ hybridization in both embryos and adult retinal tissue. As further confirmation, pax6b splice-site morpholinos were injected into one-cell Tg[pax6b:GFP] embryos. Reduction in the percentage of offspring expressing the GFP reporter signal in morphant versus Standard Control embryos indicates that knockdown of pax6b was successful.
Poster Presentation

*Synthesis of a New Nickel (II) Complex*

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Kateri Chabot
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Various methods of reducing CO2 emissions or capturing and sequestering CO2 have been proposed. Catalyzed reductions of CO2 into chemical fuels or chemical feedstocks reduce the need for CO2 sequestration and increase availability of useful organic compounds. This summer, we sought a method for synthesizing a new organometallic compound from the ligand 4,4'-Di-tert-butylbiphenyl-2,2'-bis((2-hydroxy-3,5-di-tertbutylphenyl)amine). Once synthesized, we will study the kinetics of reactions with this compound and hydrazobenzene to understand the structure of the molecule and assess the usefulness of this compound as a potential catalyst.
Poster Presentation

*Investigating the effects of osmolytes on the folding of the preQ1 riboswitch*

Qian Hou  
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Riboswitches are regulatory non-coding RNAs found in the 5’-untranslated regions of many bacterial messenger RNAs (mRNAs), and are composed of an aptamer domain and a downstream expression platform. Riboswitches control gene expression through transcription attenuation or inhibition of translation initiation by modulating the folding and conformation of the aptamer domain in response to ligand binding. Previous single-molecule FRET (smFRET) studies on riboswitches predominantly focused on the stabilization effects of metal ions and ligand on the structure and conformational dynamics of RNA. The purpose of my summer research is to investigate the effect of urea on the conformation and structural dynamics of the Bacillus subtilis (Bsu) preQ1 riboswitch by smFRET microscopy. Previous smFRET study on the Bsu riboswitch showed that it exists in mid-FRET and high-FRET states that correspond to pre-folded and folded (pseudoknot) conformations. We found that in the absence of Mg2+, the increase in urea concentration steadily lowers both high-FRET (docked state) and mid-FRET (undocked state) efficiencies for ligand-bound form of preQ1 riboswitch, and also significantly shifts the population towards the undocked conformation. Kinetic analysis of smFRET traces shows that urea destabilizes the folding process by a gradual decline in the docking rate of preQ1 riboswitch upon the addition of urea and an increase in the undocking rate. Our results also demonstrate that urea renders the mid-FRET state into an extended and broad conformational ensemble while the high-FRET state is relatively less affected. In the presence of Mg2+, the riboswitch behaves in a similar but more complex manner, suggesting a competing interplay between the two solutes. Future emphasis will be placed on the probing the competition between urea and Mg2+, and how Mg2+ concentration influences the denaturation process.
Oral Presentation

Study of the pure double folding optical model for 100 MeV/u deuteron scattering

Kevin Howard
Darshana Patel
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The centroid energies of the giant monopole resonance (GMR) in nuclei are important because they are directly related to the nuclear incompressibility, an important quantity in the nuclear equation of state. It is necessary to examine the properties of the GMR in nuclei far from stability using advanced experimental techniques. The optical model for deuteron scattering is important from the point of view of performing these studies in inverse kinematics. Most studies on deuteron optical potentials have been done at lower energies and using the phenomenological optical model. However this model has been shown to overestimate the cross-sections for the low-lying discrete state. Recent developments in theory allow for the optical model real and imaginary volume potentials to be calculated using a double folding model with the help of the computer code dfpd5. For the first time these calculations are used to model the elastic and inelastic angular distributions in $^{28}$Si, $^{58}$Ni, and $^{116}$Sn nuclei. The experiment was performed at the Research Center for Nuclear Physics, Osaka University, Japan, using a 100 MeV/u deuteron beam. Results of the analysis will be presented.
Oral Presentation

Modal noise mitigation in optical fibers with small circular diameters

Patricia Huestis
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“Modal noise” occurs when light propagating through an optical fiber excites specific modes and creates an interference pattern; its effects can introduce spurious Doppler shifts when acquiring precise radial velocity (RV) measurements of nearby stars in search of extrasolar planets. The severity of modal noise worsens as the wavelength of light increases and also as the optical fiber core diameter decreases. iLocater, a planet-finding instrument currently being developed for the Large Binocular Telescope, will be the world’s first diffraction-limited Doppler spectrometer. It aims to work in the near-infrared (NIR) and use optical fibers with core diameters no larger than 50 microns, so modal noise could be especially problematic. This paper discusses an inexpensive solution to reduce modal noise in 50 micron core optical fibers at a wavelength of 632.6 nm, though is also applicable to multi-mode fibers of various sizes. Our preliminary experimental results demonstrate that circular fiber motion is an effective method for spatially smearing out the modal noise pattern in small core fibers. Such mitigation schemes will aid in the design of a mechanical agitator for iLocater that will ameliorate modal noise patterns. In doing so, we will be able to achieve the first RV measurement precisions below 1 m/s in the NIR region. Ultra-precise RV measurements will allow for the detection and study of “Earth-like” exoplanets orbiting in the habitable-zone around nearby M-type stars, ultimately giving us clues to how our own planet formed and developed.
Along with habitat loss, a shift in temperature due to climate change is a key contributor to the recent extinctions of endangered species. Many populations of the Karner blue butterfly, *Lycaeides melissa samuelis*, have become critically endangered to the point of extinction in the past few years, due to a multitude of factors. Thus far, climate change has been of unknown impact on the survival of the Karner, but the Karner is an ectotherm, meaning that it is easily affected by a changing habitat climate. This study attempts to comprehend the effects of a projected temperature increase due to climate change on the development rate, body weight, and survival rate of *Lycaeides melissa samuelis*. Through data collection, the study may assist in predicting the effects of future temperature changes on the survival of dwindling Karner populations. Karner blue butterflies were raised and bred in captive environmental chambers at two separate temperatures (18°C and 26°C) from the egg stage to the adult stage. Hatch dates, pupation dates, eclosion dates, and death dates, along with regular interval masses were recorded. Results suggest that an elevated temperature leads to more rapid development at a lower mass and a lower survival rate. Climate change may be one of the contributing factors to the dwindling survival of the Karner species. This experiment also suggests the negative impact of a rising climate on other temperate insect species.
Scanning tunneling microscopy (STM) studies of ferrocene carboxylic acid (FcCOOH) strongly suggest that hydrogen-bonded clusters containing 5 or more FcCOOH molecules are present in solution under some conditions. Infrared (IR) spectroscopy of FcCOOH should give more insight into the size and number of clusters, based on analysis of the C=O and O-H stretching regions and comparison of experimental and calculated IR lineshapes. Deuterated acetone is a favorable solvent for FcCOOH as it is aprotic, yet allows the molecule to quickly exchange its hydrogen for a deuterium in solution; the OD stretch in FeCOOD is then spectrally separated from other vibrations. Varying the concentration of FcCOOH from very dilute to saturated solutions will allow for examination of the correlation between concentration and cluster quantity and size.
Overshadowing the size of galaxies is the cosmic web, which is composed of sheets, walls, and filaments regulate galaxy evolution by the accreting mass into galaxies via filaments. In an effort to further understand the evolution of galaxies, we first study filaments and devise an interactive analytical model for disk galaxies with accurate inflow and outflow rates of matter. Using accretion rates and feedback rates from different regions in the Galaxy, it is now possible to model and predict galactic behavior for a galaxy with similar mass and morphology as the Milky Way. Other models model feedback or accretion processes numerically and in greater detail. Here we consolidate the rates to make one single model for the galaxy as a whole. In this model, we take the rates from other papers and use them to calculate the total mass flowed energy used, distance travelled, and current location of the gas from the following parameters: change in time, redshift value, morphology of the galaxy, and type of active galactic nuclei (AGN) the galaxy has at its center. Although, we have just begun to make this detailed model, it will serve as the foundation for future work to be done to further understand galaxy evolution.
Articular cartilage and tendon damage is difficult to noninvasively image because soft tissue has low X-ray attenuation. Gold nanoparticles (AuNPs) have high X-ray attenuation and can be functionalized with positively charged molecules to target negatively charged glycosaminoglycans (GAGs), which are exposed when tissues are damaged. AuNPs were synthesized and functionalized with poly-L-lysine (PLL) or poly(ethyleneimine) (PEI) molecules, both of which are positively charged. Bovine patellar cartilage and Achilles tendon samples were prepared. Using a drop tower cartilage samples were impacted to create articular surface fissures and damage throughout the depth. Other cartilage and tendon samples were manually damaged on the surface using a scalpel incision. Samples were either dyed with India ink or soaked in functionalized AuNP solution overnight and imaged.

As-synthesized PLL-AuNPs and PEI-AuNPs exhibited near neutral pH and high positive zeta potentials. Functionalized AuNPs were stable as-synthesized but less stable in the presence of tissue samples, especially when concentrated for X-ray imaging. In cartilage samples where functionalized AuNPs remained stable, the AuNPs appeared to target the undamaged articular surface but not the damage site. In tendon samples, the AuNPs targeted the surface damage (Fig. 1). This difference may be due to a difference in the GAG release mechanisms of each tissue. Future work will focus on improving the stability and concentration of functionalized AuNPs. AuNPs may be a noninvasive solution to image the GAG distribution and damage in articular cartilage. This could improve diagnosis of diseases such as osteoarthritis resulting in fewer debilitating joint injuries.

Figure 1: Photographs of (a) the top surface of articular cartilage (6 mm diameter) damaged by scalpel and labeled by PLL-AuNPs and (b) the cross-section of tendon (9 mm wide) damaged by scalpel and labeled by PEI-AuNPs
Microbial ecology requires a fundamental understanding of microorganisms’ eco-physiological traits, where traits refer to the environmental responses and contributions of microorganisms to the environment. Co-variations in these set of traits are referred so as to trade-offs. Preliminary growth kinetics results in our laboratory allowed the establishment of a trade-off between resource acquisition and the competence of bacteria to grow at a maximum rate. Bacterial cell growth is controlled by the rate of active transport of a limiting substrate, and thus, association between cell growth and specific substrate transporters is established. A connection among bacterial growth kinetics, defined in terms of \( \mu_{\text{max}} \) and \( K_s \), and cell growth is then to be determined. Subsequent relationship between bacterial kinetic capabilities and genetic information based on substrate transporters is fundamental to further understand bacterial lifestyles. To generate traits-level understanding of bacterial ecology, a combination of classical microbiology methods, whereby bacterial specific growth rate was monitored over time by measuring the optical density of the cultures at different substrate concentration to obtain kinetic data (i.e. \( \mu_{\text{max}} \) and \( K_s \), based on Monod’s model), data analysis and comparative genomics was exploited. This study verified the trade-off between the ability to acquire glucose and phosphorous and the competence to grow at a maximum growth rate for six freshwater bacterial strains. A connection between freshwater bacterial transporters and lifestyle to establish a model that allows quantification of microbial growth kinetics in order to predict microbes’ lifestyles from their genetic background was consequently ascertained.
Characterization of matrix metalloproteinase-8 inhibitors for the treatment of sudden inflammatory response syndrome

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Matrix metalloproteinases (MMPs) are a class of enzymes that degrade the extracellular matrix of multicellular organisms. Overexpression of MMP-8, an enzyme responsible for breaking down extracellular collagen structures, plays an important role in mediating sudden inflammatory response syndrome (SIRS): it contributes to the lethality of SIRS by breaking down structures critical to the blood-cerebral spinal fluid barrier. Thus, MMP-8 has been proposed as a potential drug target for treatment of SIRS. Compound 1 has been reported as a highly selective inhibitor of MMP-8 and MMP-13. Four derivatives of compound 1 (compounds 2-5) were designed, synthesized, and evaluated for enzyme kinetics, plasma stability, metabolic stability, and in vivo pharmacokinetics. The compounds showed improved inhibition of MMP-8 and were stable in plasma and rat liver S9. The compounds had low to moderate clearance from plasma. Compound 3 is currently being evaluated in a mouse model of SIRS.
Metabolites are small molecules, such as various amino acids, organic acids, carbohydrates, ketones, and aldehydes, which are the final products of cellular regulatory processes. Metabolite levels profoundly signify the ultimate response of biological systems. The science of metabolomics refers to the identification and quantification of metabolites found in an organism, and is the fastest growing field in relation to biomarker discovery for disease diagnosis. Various biological specimens, such as body fluids, including urine and blood, cells, and tissues are being used for metabolomic analysis, which provides a plethora of metabolite rich information. These biological samples are generally analyzed by nuclear magnetic resonance (NMR) spectroscopy. However, subtle physiological changes between urine samples, such as pH variance and salt concentration differences, can cause changes in the chemical shifts of metabolites across the NMR spectra of multiple samples, interfering with multivariate statistical analysis. Therefore, peak alignment, the identification, and quantification of metabolites are still complex procedures, as there is an inherent lack of consistency across samples. In an effort to overcome this problem, we propose a simple separation procedure, to be used with urine samples, which precipitates salts and proteins in urine samples that can cause chemical shift variance while leaving metabolites unchanged (Figure 1). In this approach (Scheme 1), native urine samples were combined with decanoic acid at high temperatures, dried, and then suspended in D2O. Subsequently, 1D 1H NMR measurements were carried out with water presaturation. The resulting spectra of the various urine samples showed consistent chemical shift values for metabolites in each spectrum. This procedure greatly reduced the chemical shift perturbations across the different urine samples, allowing for more accurate multivariate statistical analysis, identification and quantification of urine metabolites, which can be used routinely in NMR-based metabolomic analysis of urine samples, most importantly in biomarker discovery for cancers.
Oral Presentation

*Beamline optimization for Long Baseline Neutrino Experiment*

Yi Jia  
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One of the physics goals of Long Baseline Neutrino Experiment (LBNE) is to measure CP violation in the neutrino sector and to determine the mass hierarchy. This summer, we work on various simulations to explore an optimal design of neutrino beamline. Such an improved beam is expected to achieve by maximizing events at first and second oscillation maxima while minimizing high energy tail that produce backgrounds, eventually leading to better resolution of the CP phase. The studies were done by advanced tool G4LBNE combined with Fermilab Grid. To determine the optimizing construction with most potential to obtain our physics goals, different structures and parameters, such as adding a plug, beam power and horn current, are compared to underline their effects. The simulation results show that a plug can play a significant role to enhance our spectra. As a powerful simulation tool, Fast Monte Carlo provides detailed information including efficiencies, purities and detector response for us to understand the experiment.
Graphene oxide is a matrix of carbon rings with carboxyl and hydroxyl functional groups attached throughout. When paired with semi-conductors and metal nanoparticles, graphene oxide can be used as a smart material to both sense and shoot target organic molecules. Graphene oxide interacts with and immobilizes target molecules through dipole-dipole and van der Waals forces with various functional groups. The focus of this project was to study the concentrating effect of graphene oxide. To test these interactions, we ran adsorption experiments between graphene oxide and crystal violet dye. Because crystal violet is a charged molecule, the strength of its intermolecular interactions and resulting adsorption on the graphene oxide surface can be tuned by varying the pH. This study will help optimize our multifunctional sense and shoot films. The centrifuge experiments helped provide information on quick adsorption properties of graphene oxide, whereas kinetics experiments provide information on the long-term adsorption properties of graphene oxide over a span of 48 hours. These experiments were run at various pH values to test how a change in charge of functional groups on graphene surface affects adsorption of target molecules.
Scientists can almost never recreate the same computational experiment twice which often leads to large gaps in knowledge. Reproducibility in computational sciences is hard due to the numerous dependencies between software, data and hardware, and lack of good tools to define computational steps (workflow tools) each experiment requires. In order for scientist A, Alice, to send her experiment to scientist B, Bob, Bob must install and run the executable, the exact version of pip, various software packages, and a version control software as well to deal with file installation issue/corruption, etc. Along the way something will break causing the experiment to fail to execute.

This is a critical issue for DASPOS scientists who need to preserve their experiments for future scientists to examine when the technology is better. Several software technologies, such as Reprozip and CDE are available to package the experiment and rerun the experiment in a sandboxed environment. These programs capture the provenance (data, workflow and environment) by tracking executables of the experiment via p-trace or systemtap. However, there are several drawbacks to these technologies. They are oftentimes difficult to install and use, only operate in Linux environments and are kernel dependent. Due to kernel dependencies, the package will fail to execute on Bob’s side unless it is an exact match to the Alice’s kernel environment.

A proposed solution to eliminating kernel dependency is to use Docker. Docker is a light, portable container which allows to run other applications (ie Reprozip, CDE) inside Linux containers (LCX). This allows the dependency to move from the virtual machine specific kernel to Docker - a much more feasible solution to save.
Poster Presentation

*Tandem Reversible Irreversible Cross-linking (TRIC): A Novel Method for Examining Localized Protein-Protein Interactions During Eukaryotic Gene Transcription*

Micah Katz
Amanda Dugan
Advisor: Anna Mapp, Dept. of Chemistry, University of Michigan

The formation of multi-protein complexes is essential to a myriad of biological processes, including gene transcription, cell signaling, and the maintenance of protein homeostasis. While in vitro techniques such as co-crystallization and pull-down assays have allowed for the investigation of high affinity protein-protein interactions (PPIs), in vivo studies of moderate and transient affinity interactions have proven more challenging to examine. Herein we employ the genetic incorporation of photoactive unnatural amino acids into protein surfaces in order to covalently capture the moderate and transient affinity interactions that occur in vivo during eukaryotic gene transcription. Furthermore, we combine this irreversible covalent cross-linking method with reversible formaldehyde cross-linking to obtain detailed mechanisms of the assembly of transcriptional machinery at specific gene promoters. We demonstrate the utility of this method, termed tandem reversible-irreversible cross-linking (TRIC), by investigating the mechanism of recruitment of the TFIID subunit TBP to the GAL1 promoter by transcriptional activators VP16 and Gal4. Different laboratories have purported various models of TBP recruitment by VP16, both direct and indirect, and equally conflicting reports exist for Gal4’s proposed recruitment. By incorporating the photoactive unnatural amino acid, p-benzoyl-L-phenylalanine (Bpa), into the transcriptional activation domains (TADs) of VP16 and Gal4 and utilizing the novel TRIC method, we establish a first step in obtaining a detailed picture of the PPI network at the gene promoter that gives way to transcription initiation.
Investigation of Thermal Rectification during Transient Heat Conduction

John Kearns
Advisor: David Go, Dept. of Aerospace and Mechanical Engineering, University of Notre Dame

Thermal rectification is the phenomenon of asymmetrical heat flow through a medium. More clearly, a thermal rectifier is a material for which the magnitude of heat flow for a given temperature difference depends on the orientation of that difference; the rectifier acts as a conductor for one orientation and an insulator when the temperature difference is reversed. Understanding of the phenomenon of rectification may lead to improvements in energy efficiency for a number of applications. However, rectifier performance is typically only evaluated under steady state conditions instead of transient conditions, which are more representative of most applications. In conduction, rectification can occur in composite materials due to the temperature dependence of the materials’ thermophysical properties. While all heat conduction depends on a material’s thermal conductivity, only transient heat conduction depends on its thermal diffusivity. To investigate transient rectification effects, as well as determine the role of thermal diffusivity, analytical solutions to various permutations of the heat equation are determined and studied. The primary goal of this research is to determine if a relationship exists between the degree of rectification that occurs during transient and steady heat conduction for a given system. If such a relation exists and is determined, it will enable improved design of rectifying structures and ultimately lead to improved energy efficiency for a variety of applications.
In 1994, the NNDC revolutionized nuclear research by providing a colorful, clickable, searchable database over the internet. Since then, web technology has evolved dramatically, but the NNDC’s user interface remains largely unchanged. Our project, the Notre Dame Nuclear Database, aims to provide researchers with a more comprehensive, interactive, and broadly searchable body of data. The database can be searched by an array of filters which includes metadata such as the facility where a measurement is made, the author(s), or date of publication for the datum of interest. The user interface takes full advantage of HTML, a markup language that encodes the vast majority of webpages, CSS (cascading style sheets which define the aesthetics of the website), and JavaScript, a programming language that allows our website to process complex data. The server-side technologies used to power the webserver are MySQL, a relational database management system, and Python, a high-level programming language that we use to access and return data. In addition, our team has developed a first-of-its-kind command-line interface that allows users to interact with the database directly on their local machines without having to open a web browser. For example, users can request to download specific, pre-parsed content in numerous data formats with a simple command. This is possible through the use of a standardized API (application programming interface) that relies upon well-defined filtering variables to produce customized search results. Our database also offers an innovative chart of nuclides utilizing scalable vector graphics (SVG) to deliver researchers an unsurpassed level of interactivity supported on all computers and mobile devices (including touch features such as scrolling and pinch-zooming). Our team intends to make (ND)2 an open source project, and we will present a functional demo of our database at the conference.
The topic of research for my RET (Research Experiences for Teachers) project is Water Filtration and Purification through Functional Nanofiltration Membranes. I have worked with Siyi Qu, a graduate student who works under Dr. William Phillip. The purpose of this study is to reduce water stress and increase the Earth’s available water supply. These membranes help with filtering unwanted particles from water. Water filtration might seem like a pretty easy concept to understand, but this is water purification and desalination at the nano-level. This filtration is done by making copolymer membranes with microscopic pores. These pores typically range from 0.01 to 0.001 microns in size. The membranes need to be robust with high flux (the rate at which water permeates) and good selectivity (filtering necessary particles). My role in this research is to carry out the transport and rejection tests for the copolymer membranes that Siyi Qu has developed. I run solutions, usually dyes, through these membranes during the transport tests, checking for flux and permeability. The transport test is conducted by placing the membrane into a stir cell. Air is then passed through the cell to push the water through. The water passes through a tube and into a vial which is placed on a scale. I also conduct rejection tests on the solutions to find out the percentage of the particles which the membranes have filtered. The rejection test is conducted by using ultraviolet-visible (UV-vis) spectroscopy. UV-vis spectroscopy compares the absorbance of light from wavelength data from concentration of the sample to the data from a calibration curve formed by carefully prepared set of dye solutions.
Advances in cellular imaging have prompted the research of new dyes that can be used to detect and characterize nucleic acids as well as in nuclear imaging. This has raised the demand for investigation of chromophores that are not only highly fluorescent, but also non-damaging to live cells. In particular, chromophores should be non-toxic and fluorescent at wavelengths that are not harmful to the nuclei or cell. Recent studies of specific fluorescent DNA-binding complexes demonstrates the ability of these molecules to be excited at longer, less damaging wavelengths, while giving significantly improved contrast ratios. Specifically, molecules that demonstrate two-photon absorption may allow excitations even further into the infrared wavelengths. We have been focusing on chromophores for imaging in which two-photon excitation is possible. This study focuses on the photophysical properties of eight compounds with potential application as fluorescent nuclear chromophores. These compounds are of interest because of their ability to be excited at longer wavelengths, and their potentially high two-photon cross sections. The main variations among the compounds (donor-acceptor-donor motif) are conjugation length and different aromatic electron acceptors. Their structures include a pyrimidinol, difluoroboron diketonate, dicyano pyran, and pyrimidine as the central electron accepting aromatic ring. The studies performed on these compounds include steady-state measurements, two-photon absorption spectroscopy, and fluorescence upconversion spectroscopy. All compounds demonstrate modest two-photon absorption cross sections. However, the pyrimidine based compound showed an impressive cross section, and may be tailored further for use in cell imaging.
Mosquitoes rely on their sense of smell to find hosts for feeding, which includes plants for sugar and animals for blood meals. A divergent family of proteins, Odorant Receptors (ORs), expressed on the dendrites of Olfactory Receptor Neurons (ORNs), mediates the olfaction. The OR families among Culex, Aedes, and Anopheles mosquitoes share little homology that can be attributed to the different hosts they exploit for blood feeding, distinct habitats, and oviposition sites. One common trait among these three mosquito genera is their propensity to seek sugar from plants for their very survival. We hypothesized that there could be a few conserved ORs that mediate this shared behavior. Indeed there are a handful of the conserved ORs. One such highly conserved receptor is OR2 that is over 70% conserved among the three genera. Using the Gal4/UAS system to express mosquito ORs in Drosophila and exposing these flies to odors from attractive plants resolved on a gas chromatogram (GC), our group previously determined that OR2 from Cx. quinquefasciatus (CquiOr2) responds to two phytochemicals, benzaldehyde and indole.

Anopheles gambiae, the major vector of malaria, preferentially feeds from Lantana camara and Parthenium hysterophorus plants for sugars. Using flies that express AgamOR2, here I demonstrate that there are five biologically active compounds in P. hysterophorus odors and two in L. camara. I am in the process of chemically identifying these constituents using GC-mass spectrometry. These results demonstrate that a few constituent chemicals from P. hysterophorus and L. camara indeed elicit strong olfactory responses from AgamOR2. It is interesting to note that P. hysterophorus also has antimalarial properties.

Figure 1: Anopheles gambiae odorant receptor (AgamOR2) responds to constituent odorants from P. hysterophorus plant. Single unit recordings from the neuron expressing AgamOR2 show excitation to the plant constituent odorants as they elute from a gas chromatogram.
Presented is a search for the Higgs Boson produced in association with top-quark pairs and decaying to hadronic taus. This project seeks to optimize signal sensitivity (signal-to-noise ratio) of previously published analysis using new techniques. Improvements in tau identification, multivariate selection, and event categorization were studied. A maximum likelihood technique was used to generate expected limits on the sensitivity of the analysis for observing ttH production. The results use the standard model expectation for ttH production where $m_H=125.6$ GeV.
As part of immune defense, macrophages in the human body produce nitric oxide (NO) in order to kill off invading pathogens. Bacteria that express flavodiiron nitric oxide reductases (FNORs) are able to detoxify the NO by reducing it to N2O, allowing them to proliferate. Despite the importance of these enzymes in bacterial pathogenesis, the mechanism of FNORs is not currently known. Our group recently reported that upon two-electron reduction, the FNOR model complex [Fe2(BPMP)(OPr)(NO)2](BPh4)2 produces N2O, suggesting that the enzyme could use a similar pathway to detoxify NO in vivo. In order to demonstrate that a diiron motif with cis NO moieties is required for efficient N2O production, model complexes employing derivatives of the ligand BMPA-PhOH (N-(2-hydroxybenzyl)-N,N-bis(2-pyridylmethyl)amine) have been synthesized and characterized using UV-Visible, IR, and EPR spectroscopies as well as X-ray crystallography. These complexes can exist in solution as monomers or as phenolate-bridged dimers (shown below), depending on the substitution of the phenolate group of the ligand. In contrast to the BPMP model complex, which produces N2O rapidly and quantitatively upon reduction, the BMPA-PhO model complexes initially disproportionate upon reduction to form a ferrous complex and a dinitrosyl iron complex (DNIC). N2O formation occurs only slowly and in low yield.

Figure 1. Crystal structure of the dimeric model complex [Fe2(BMPA-PhO)(NO)]2−.
Cardiac arrhythmias are a set of electrophysiological disorders of the heart that detrimentally disrupt the heart’s normal sinus rhythm. Atrial fibrillation, a particular type of arrhythmia, affects approximately 2.3 million adults in the USA and may increase one’s risk of potentially deadly stroke five-fold. The current standard of care includes useful catheter ablation procedures, which involve the direct application of energy to the heart in order to destroy the problematic cells that are the electrical sources of the disease, which include both cardiac myocytes and sympathetic nerve terminals. Currently, however, this procedure can destroy the surrounding spectator tissues in the ablated region, causing significant side effects and limiting the amount of energy that can be safely applied during the surgery. Because of this, there is a significant need for a safer, targeted approach to ablation therapy that can spare surrounding tissues. This ongoing project, which is a translational collaboration between Dr. Kopelman’s lab in the Department of Chemistry, Dr. Raffel’s group in the Department of Radiology, and Dr. Kalifa’s lab in the Department of Internal Medicine, aims to achieve the selective ablation of specific tissues in vitro by designing a targeted and functionalized polyethylene glycol nanoparticle for use in photodynamic ablation therapy (PDT). The nanoparticles are purposely built with specific targeting, crosslinking, and reactive oxygen species producing moieties all working together to effect specific destruction of a chosen cell type. Chlorin-E-6 (Ce6), the photosensitive dye used in this project, produces many locally destructive reactive oxygen species when exposed to red light. When attached to the nanoparticle scaffold, it kills only those cells to which the larger nanoparticle is targeted and only in the region of illumination. Thus, this potential approach is targeted at both the molecular and surgical/illumination level, which promises marked improvements over current techniques and, conceivably, better patient outcomes. This summer investigation focused primarily on the synthesis and characterization of myocyte targeted nanoparticles. We also synthesized a custom meta-iodobenzylguanidine conjugated nanoparticle so as to target cardiac sympathetic nerve terminals, which help perpetuate arrhythmias. Later on in a future experiment this fall, we will aim at analyzing in-vitro myocyte and sympathetic nerve terminal PDT results using these drugs. In preparation for future in-vivo testing of the targeted ablation procedure on nerve tissues, this work so far has established this approach as feasible and worthy of additional study. Hopefully, this will lead to an eventual application to human patients.
Developing nitrile Stark probes of plasmonic fields

Daniel Kwasnieski
Advisor: Zachary Schultz, Dept. of Chemistry and Biochemistry, University of Notre Dame

The local electric field environment of plasmonic nanostructures is of particular interest both to science and industry, where these nanoscale properties find many applications. However, direct assessment of these fields is difficult, and the common practice of indirectly inferring the field strength from signal intensity has certain pitfalls. A recently reported method identified the vibrational Stark effect as capable of directly measuring the local field in the gap junction of a nanoparticle dimer from frequency shifts in a Raman vibrational mode of CO. Expanding on previous work in our lab which investigated CN adsorbed to Au to image electric fields, here we study CN and two thiolated nitrile-capped probe molecules on Ag SERS substrates as potential Stark reporters. Efforts were made to calibrate the observed nitrile stretching frequency as a function of the incident laser power. From these studies, the CN frequency is observed to correlate with electric fields, but further study is needed to quantify this effect.
Poster Presentation

_Catalytic Fast Pyrolysis of Lignocellulosic Biomass with Manganese-Incorporated MFI & MTW Zeolite Catalysts_

David Lawrence  
Gregory Neumann  
Advisor: Jason Hicks, Dept. of Chemical and Biomolecular Engineering, University of Notre Dame

Manganese-incorporated zeolites were synthesized using two different structure directing agents to produce MFI and MTW type zeolites. Tetrapropylammonium hydroxide (TPAOH) was used as the organic template to produce MFI, while tetraethylammonium hydroxide (TEAOH) was the template for MTW. Using a hydrothermal method, manganese (III)-acetylacetonate was incorporated within the two zeolite types. These catalysts along with the MFI and MTW catalysts without Mn were studied for the catalytic fast pyrolysis of biomass. Corn stover and glucose were used as the lignocellulosic biomass. They were pyrolyzed and then passed through the catalyst and analyzed by gas chromatography and mass spectroscopy to determine the type and abundance of products. Selectivity of the products was calculated and compared between the catalysts studied.
Accelerating the Analysis of SANS of Superconducting Vortex Lattices

Allan Leishman
Advisor: Morten Eskildsen, Dept. of Physics, University of Notre Dame

Graphical Reduction and Analysis SANS Program (GRASP) is a program developed in MATLAB™ for the analysis of small-angle neutron scattering (SANS). The software engages the user through a series of GUI’s which allow the user to view and analyze their data in a straightforward manner. Of particular interest to this group is the ability to fit multiple Gaussian peaks to the data files with relative ease, which can be used to characterize the superconducting vortex lattice states in MgB2. However, one weakness of GRASP is the inability to analyze large collections of files quickly, as they all must be manipulated individually and fit by hand. This problem has been resolved through the creation of Multi-File Fitter (MFF), a user module designed to analyze large sets of files rapidly and export the fit parameters in a simple manner. MFF has greatly accelerated the analysis process, from a matter of days to a matter of minutes.
Poster Presentation

*New Avenues for Iron-Catalyzed Dehydrogenative Cross-Coupling Reactions*

Qiuhan Li  
Emilia Groso  
Advisor: Corinna Schindler, Dept. of Chemistry, University of Michigan

The biaryl structural motif is an important feature found in many functional materials such as light-emitting diodes (LED) and liquid crystals. It is also present in many biologically active compounds. This motif is typically obtained via C-H activation and cross-coupling methods; however, these methods typically require the prefunctionalization of the coupling partners and subsequent removal of the activating groups. Inspired by the role of iron-containing P450 enzymes by which *M. tuberculosis* uses to catalyze oxidative coupling reactions, we aim to use transition metal complexes to catalyze the dehydrogenative cross-coupling reactions. This novel method will eliminate the need for lengthy prefunctionalization. Currently, the transition metals we are exploring are iron, chromium, manganese, copper, vanadium, and ruthenium. The ligands of interest are salen and salan ligands. Based on our preliminary phenol coupling catalyst evaluation results of 2,4-di-tert-butylphenol, iron-containing and vanadium-containing salen complexes give us a 60%-70% yield. After building up our ligand library and transition metal complex library, we are planning to conduct more comprehensive catalyst evaluation to test the ability of those complexes and to examine the substrate scope. Once we have viable transition metal catalysts, we can apply them to natural product synthesis. Specifically, we are interested in applying these catalysts towards the synthesis of mycocyclosin and similar substrates, which can potentially act as novel *M. tuberculosis* inhibitors.
The control of DNA (deoxyribonucleic acid) on silicon substrates is an important pre-step for application of DNA in the computer and semiconductor industry. Using DNA nanostructures as a way to pack information onto microelectronic chips has the potential to meet high processing demands. The goal of this research was to explore the limits of thermal stability of DNA origami attached to an APTES monolayer on a silicon substrate. The data obtained quantified the survival of these nanostructures at extreme temperatures. The procedure involved taking water contact angle measurements of DNA nanostructures on APTES at room temperature before and after heating in a tube furnace. Versatility of DNA origami designs are attributable to the self-assembly properties of DNA, which can be instructed to form 2-D and 3-D shapes. These studies were performed using 2-D rectangular DNA origami. The atomic force microscope was used to obtain images for analysis. Water contact angles and heating of the APTES at 150° to 650° were repeated in two experiments. The results show that 85 % of the DNA origami folded correctly with an average height of 2.57 nm ± 0.75 nm. The APTES samples were smooth and clean with an average of 2.23 nm in roughness. The thermal stability of APTES did not decrease until 350°. The DNA was stable at 150°, and was not stable at 250°. This data show the advantages and applicability of silicon chips that have been processed with CMOS (complementary metal oxide semiconductor) compatible processes as solid support for measurements of thermal stability in molecular films at extreme temperatures.
Search for Gamma-Ray Sources from a Measurement of the Muon Angular Distribution with High Statistics

Chuanhong Liu
Advisor: John Poirier, Dept. of Physics, University of Notre Dame

Project GRAND is an array of proportional wire chamber stations which detects secondary muons produced by cosmic ray primaries. It has been used to detect muons since 1995. In this report, 6.5 years of data has been analyzed in order to construct a high statistic angular map of muon flux in celestial coordinates (right ascension, declination) and in solar coordinates (solar hour of day EST and declination). We search for muons in coincidence with gamma-ray sources with GRAND using data from 1 Jan 2007 to 30 Jun 2013.
The study of proteins and peptides derived from complex organisms is always hampered by the complexity of samples from which they originate. In recent years, bioorthogonal chemical approaches have been developed so that certain molecules or classes of molecules can be enriched from these complex samples making them more amenable to thorough study. This approach has allowed researchers to incorporate unique functional groups into proteins and peptides of interest so that they can be selectively reacted with tags for downstream labeling or enrichment. The incorporation of chemoselective functional groups for bioorthogonal labeling has great potential for imaging and for selectively controlling individual proteins in living cells. Recently, metals have been used to catalyze reactions forming new carbon-carbon bonds in biological samples. For example, palladium-catalyzed cross-metathesis has been explored for its chemoselectivity and utility in biological systems. Proteins carrying allyl sulfides or allyl selenides react with allyl alcohols in the presence of a free phosphine. Suzuki cross coupling is another palladium-catalyzed reaction in which the coupling partners are an aryl boronic acid with an aryl halide. Its broad scope and utility was highlighted by the awarding of the 2010 Nobel Prize in Chemistry to Akira Suzuki, among others, for their effort for the development of palladium-catalyzed cross coupling reactions in organic synthesis. We are using the Suzuki cross coupling reaction as part of our project, as it has been used previously in protein chemistry with success. We demonstrate here its use specifically in the development of chemical protein and peptide probes. We have successfully incorporated bromophenyl moieties into various proteins and peptides and coupled them to probes containing phenyl boronic acid or trifluoroborionate groups. We have also synthesized a fluorescent dye containing an aryl boronic acid group for covalent labeling and detection of bromophenyl-adducted proteins.
To study the nuclear structure of deformed nuclei, in particular, 0+ excited states in several gadolinium isotopes, we plan to perform ($\alpha$, n) and ($\alpha$, 2n) reactions on enriched samarium targets utilizing coincidence and time of flight techniques to measure conversion electrons, gamma rays and neutrons. As a preliminary experiment, natural samarium targets were used. Alpha particles, 16-21 MeV in energy, were incident upon a series of four natural samarium targets with the primary aims to measure cross sections of the selective ($\alpha$, n/2n) channels and test the targets. Data were collected via an Internal Conversion Electron Ball array (ICEBall) containing six Si(Li) detectors and accompanying neutron and gamma-ray counters. Spectra were observed in ICEBall from electrons emitted from a range of reaction channels both in ground state and excited states of gadolinium. The focus was set on ($\alpha$, n/2n) channels that were more easily observed and identified with conversion electron peaks emitted from gadolinium-154, 156 and 157. We will present the results on conversion electron emission cross-sections as well as neutron and gamma fluxes and compare with TALYS calculations. These data give insight for performing future experiments that will use enriched targets so as to allow optimum beam energy for particular reaction channels while maintaining a neutron flux that is non-destructive for HPGe detectors.
An emerging, highly interdisciplinary field in physics has been created which combines plasma technology with biomedical applications. Plasma has been used for sterilization purposes and in the areas of dentistry and cosmetics but is more recently being researched for various medical advancements, including wound care and oncology. In my research project, the plasma is in the form of a non-thermal jet, which can be created under ambient conditions, which is an advantage, as it does not require a vacuum chamber for the jet to be sustained. My project is aiming to understand how the plasma jet affects the cells and to analyze the damage induced to DNA depending on plasma exposure duration. The DNA can be damaged due to the production of single strand breaks (SSB) and double strand breaks (DSB). By using agarose gel electrophoresis we are able to analyze irradiated DNA and see what type of damage has occurred, as well as the amount of DNA that remained intact during radiation. In order to enhance DNA damage, which can have benefits in cancer treatment, we use a helium plasma jet with oxygen (O2) admixture. Moreover, we try to reveal how the presence of oxygen affects the DNA. As higher concentrations of oxygen (up to .5%) are used in the helium plasma jet, we see more breakage most likely due to the formation of reactive oxygen species (ROS). ROS are known to be highly reactive and can create damage to DNA.
Rainwater is a vital part of the ecosystem, impacting vegetation, water quality, and soil chemistry, among other environmental effects. Atmospheric particles are involved in the formation of clouds and precipitation by serving as cloud condensation and ice nuclei for the condensation of water vapor. Depending on their size and chemical composition, these particles are able to travel large distances, and thus, they affect both climate change and the characteristics of precipitation. Rainwater was collected in Ann Arbor, Michigan on June 23, June 24, and July 8, 2014 to investigate the properties of the rainwater. Nanoparticle tracking analysis was to measure the particle size distribution within the rainwater samples. Ion chromatography was used to analyze the ion content (lithium, sodium, ammonium, potassium, magnesium, calcium, fluoride, chloride, nitrite, bromide, nitrate, phosphate, and sulfate) of the rainwater collected. In addition, the pH of the rainwater was measured, and ultraviolet–visible spectroscopy was to measure the absorption of the rainwater samples. Lastly, the NOAA HYSPLIT model was used to estimate the backward trajectories of the air masses arriving above Ann Arbor to determine potential source regions of the original atmospheric particles. Our results will give greater insight to the chemical components of rainwater and the effects they may have on the environment.
The WHO defines a counterfeit medicine as a drug whose active ingredient is either under dosed or completely absent. The worldwide counterfeit business was able to sell more than 200 billion dollars worth of counterfeit pharmaceuticals in the last few years. This should cause an immediate concern to those that serve vulnerable communities, such as those who serve as pharmacists, doctors, and social workers, among others. Vulnerable communities could be defined as those in which analytical resources, such as trained pharmacists or analytical instruments, are scarce. Using simple, colorimetric chemistry on a paper-based device, the Paper Analytical Devices (PADs) have been adapted to provide an inexpensive and practical method for developing countries to screen for counterfeit version of a drug. These PADs yield a quick identification of known ingredients found in genuine and counterfeit drugs and also enable the quantification of their respective active ingredient. Metronidazole was chosen to specifically validate the PAD because its common counterfeit has been reported to be under dosed. Also, metronidazole is the active ingredient in products such as Flagyl or vaginal gel which treats infections as an antiprotozoal, and this could indicate that antibiotics are added to under dosed metronidazole products in order to give a false impression of effectiveness. This project focuses on the development of this PAD, including reagent chemistry adaptation, prototype development, and the initial field testing results of 70 PADs. Along with these initial steps, there is an analysis of the field tests, indicating adequate or inadequate performance of each reagent and position of those reagents on the PAD. Instrumental analysis such as the one completed using mass spectrometry and liquid chromatography will also allow one to validate data found field testing the PADs. These steps will help one recognize the overall ability of the PAD to screen real-versus-fake and most importantly, substandard formulations of pharmaceuticals containing active ingredient, metronidazole.
A plasma is a gas consisting of free ions and electrons and plasma devices have many applications from modern compact fluorescent light bulbs to medical devices. Recently it has been shown that plasmas can be used to synthesize nanoparticles in solution, and if done in the right fluidic system, it could also potentially be used to synthesize nanomaterials in place. Using an argon gas flow to generate a plasma jet, a rich source of free electrons is created in ambient, atmospheric air that can induce electrochemical reactions. In this work, a plasma jet was generated over a droplet of diluted silver nitrate and fructose. Free electrons from the plasma were used to reduce silver ions [Ag+] present in the solution, forming a layer of silver nanoparticles where the droplet was placed. Preliminary studies showed that the nanoparticles formed a “coffee stain” where the nanoparticles are deposited at the edge of the droplet but not in the middle. Various parameters have been taken into account in order to study the impact of various variables on the synthesis and deposition process. The gas flow, droplet volume and height of the plasma were among some of the parameters controlled, while various concentrations of silver nitrate and droplet contact angles were analyzed. Currently, the silver nanoparticles formed are being characterized using a scanning electron microscope (SEM), and a mathematical model of the chemical reaction kinetics is being created.
Poster Presentation

A Patient Simulator Control System for Clinical Operators

Michael Martinez
Maryam Moosaei
Advisor: Laurel Riek, Dept. of Computer Science and Engineering, University of Notre Dame

As the demand for medical professionals has exploded in recent years, so has the demand for technology that helps students hoping to enter the medical profession become competent, capable individuals. The advancements made in medical educational technology have shifted the entire training paradigm from a “watch one, do one” approach, where students would observe a procedure once and then proceed to perform the same procedure on live subjects, to an approach that allows students to practice a given procedure several times without ever having to risk harming a person. While new technologies have enabled this transition, the tools used to drive the shift in how medical education is taught still need to be refined to better meet the demands of the industry.

Medical manikins are one such tool that is effective in the classroom, but still need to be honed. These manikins can breathe, bleed, and expel various fluids, but have static plastic faces that break the students’ suspension of disbelief. Because current technologies cannot convey the patient’s emotional, social, and physical cues (such as pain) that are so vital to interaction, students in the medical field are missing a critical component of their education. By creating an expressive face for human patient simulator systems, we hope to breathe new life into medical education technology and bring a personal element to the medical education field [1-3].

We have built an expressive robotic patient which displays live facial expressions based on both actual patients and clinical educators. This project integrates control between an existing patient simulator (Windows-based) and our bespoke robot (Linux-based). We have designed a control interface for clinical educators that exists within their existing workspace. In the future, we plan to test this new control system with our clinical partners and continue to refine its development.

Stereocilia are highly regulated structures vital for hearing in mammals. However, it is not known how their lengths are maintained. Models have been made to study possible mechanisms for actin filament maintenance in cellular protrusions, but they rely on actin treadmilling, which recent work suggests does not occur in stereocilia. We modify an existing model of motor and cargo distributions in cellular protrusions to account for the absence of treadmilling. Because there are multiple types of motors and cargo present in stereocilia, this model would need to be adapted to be predictive of specific motor and cargo distributions. Our model predicts a nonmotonic cargo distribution, with minima occurring at the base and tip. This would be a potentially suitable model for cargo that is incorporated at the tip of the actin bundle. The model is length-dependent, so more work needs to be done on mechanisms for length determination.
Poster Presentation

Visible-Light Mediated Synthesis of Constrained Cyclic-Peptides from Phenacyl Protected Cysteine Residues

Rory McAtee
Advisor: Corey Stephenson, Dept. of Chemistry, University of Michigan

Many synthetic methodologies have been aimed at constructing disulfide bonds owing to its’ significance in protein biology and short peptide therapeutics. The utility of these covalent linkages is manifest in their simple modifications between free thiols and disulfides based on the given oxidative or reductive chemical conditions. We have achieved disulfide bond formation from separate investigations of β-phenacyl-heteroatom cleavages with photoredox catalysis. Using photoexcitable Iridium complexes to catalyze single electron transfers, we have shown the reduction of the phenacyl moiety, and subsequent chemoselective cleavage of the β-heteroatom bond, resulting in the formation of a disulfide and acetophenone. In a methodology application, we wish to describe our advances toward a photocatalytic, phenacyl-(S)-cysteine cleavage approach for the construction of the disulfide bond and as an avenue of providing cyclic peptides.
Natural orbitals have been applied in atomic and molecular electronic-structure theory to increase the accuracy of calculations of observables for a many-particle system. However, unlike the electron-structure problem, the nuclear problem is translationally invariant. We created a testbed code to test the usefulness of natural orbitals as they may apply to translationally invariant problems. The relative Hamiltonian matrix of a two-particle system in one dimension is first calculated in a basis of antisymmetrized products of the harmonic oscillator eigenfunctions. The natural orbitals are then calculated for the resulting ground state, and the Hamiltonian matrix is recalculated using a two-particle basis built from the natural orbitals. The effect of basis size on the accuracy of the ground state energy calculation is explored.
Poster Presentation

Genetic analysis of podocyte development

Rachel Miceli
Paul Kroeger
Advisor: Rebecca Wingert, Dept. of Biological Sciences, University of Notre Dame

The kidneys are key organs consisting of segmented functional units called nephrons. The zebrafish embryo kidney is composed of two nephrons that share a common glomerulus. The glomerulus functions as a blood filter, and the epithelial cells of this apparatus are called podocytes. Mature podocytes are characterized by cellular extensions, called foot processes, which extend from their basal surface. These foot processes interdigitate with the extensions of neighboring podocytes and form cell-to-cell junctions called the slit diaphragm. Previously, our lab has identified and isolated two mutants: zeppelin (zep) and lightbulb (lib). Lib encodes a mutation in aldehyde dehydrogenase 1a2, which is required for retinoic acid (RA) biosynthesis, and disrupts podocyte formation during nephrogenesis. Zep mutants exhibit edema at 4 days post fertilization, and have dramatically reduced numbers of podocytes. To further characterize zep podocyte development, expression of the podocyte genes wt1a, wt1b, nephrin, and podocin was assessed at various time points of development using whole mount in situ hybridization (WISH). Furthermore, zep mutants displayed reduced wt1b-expressing podocytes at the 15 somite stage, suggesting that podocyte specification is abrogated. Recently, a morpholino knockdown of brca2 in wild-type zebrafish was found to phenocopy the zep mutants, indicating that it is a good candidate gene. Additionally, brca2 morphants display an enlarged interrenal glad similar to the zep mutants. To determine if RA acts upstream or downstream of zep, I investigated the epistatic relationship between zep and RA. RA treated embryos did not show any rescue of the mutant phenotype, suggesting that zep acts downstream of RA. Overexpression of wt1a, a transcription factor known to be required for podocyte formation, was performed to investigate if it could rescue the zep phenotype. Preliminary results indicate that wt1a overexpression is not sufficient for rescue. Future directions include determining the expression pattern of brca2 in zep and wild-type zebrafish using WISH, determining whether brca2 can rescue the zep phenotype, investigating the effect of overexpression of wt1b and a higher dose of wt1a on zep, and performing a cell death assay using the TUNEL assay or acridine orange test.
Poster Presentation

**Stability of the solar cell absorber methylammonium lead iodide perovskite during exposure in humidified air**

Pierre Alexander Miranda Herrera
Jeffrey Christians
Advisor: Prashant Kamat, Dept. of Chemistry and Biochemistry, University of Notre Dame

Sunlight is the most abundant form of renewable energy, but it is currently underutilized due to the high cost of efficient solar cells compared to fossil fuels. Methylammonium lead iodide perovskite has recently shown great promise for efficient, low cost solar cells, with efficiencies increasing from less than 4% in 2009 to 17.9% today. However, one significant problem with the perovskite absorber is the rapid degradation of its crystalline structure through the interaction with polar solvents, specifically water. For degradation analysis, techniques such as the femtosecond transient absorption spectroscopy and steady-state absorption spectroscopy were used. These techniques probe the ground and excited state of the samples and reveal the negative effects of humidity on the photophysical properties of the absorber. Also, Scanning Electron Microscopy (SEM) is used to investigate the morphological changes undergone in perovskite films exposed to humidity.
Poster Presentation

Landscape and Anthropogenic Factors Drive Blastocystis Prevalence and Genetic Variation in Balinese Macaque Populations

Sneha Modi
Justin Wilcox
Advisor: Hope Hollocher, Dept. of Biological Sciences, University of Notre Dame

*Blastocystis* is a microparasite of emerging global health interest because of its potential pathogenicity. It has been linked to gastrointestinal infections in humans, but virtually nothing is known about how it is transmitted. It is found in both humans and animals, which opens up possibilities of zoonotic transmission. Non-human primates, including long-tailed macaques are common carriers of *Blastocystis*. In this study, population genetics methods were utilized to determine genetic variation of *Blastocystis* in populations of Balinese macaques. Statistical analysis compared the prevalence of *Blastocystis* in these populations and their genetic variation to multiple landscape and anthropogenic variables. Preliminary results suggest that both landscape factors and anthropogenic factors play a role in the overall prevalence of *Blastocystis* in macaques. Specifically, the amount of water days, proximity to urban areas, and the population size of the macaques—which is affected by tourism and human food offerings to the monkeys—contribute to the overall prevalence of the parasite. Furthermore, this study indicates that human interaction may play a complex role in regards to the genetic variation of *Blastocystis* in macaques. These results are of interest because of the lack of knowledge regarding *Blastocystis* transmission.
Poster Presentation

**In vitro modification of bacterial peptides by mammalian prenyltransferases**

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Post-translational modifications are functional groups added to proteins that can alter their localization, function and activity within the cell. One such modification is lipidation, which anchors proteins to membranes, enabling the proper function and localization of a multitude of proteins. Protein prenylation, a form of lipidation, is catalyzed by protein farnesyltransferase (FTase) and protein geranylgeranyltransferase-I (GGTase-I), which add a farnesyl (15 carbon) or geranylgeranyl (20 carbon) moiety, respectively, to the C-terminus of a protein. In order for prenylation to occur, a CX_{1}X_{2}X_{3} (commonly called CaaX) motif must be present, where C is the cysteine residue that is prenylated, a is variable, and the combination of the a and X residues determine reactivity and prenyltransferase specificity, though there is significant substrate overlap. Recently, it has been shown that the human prenylation machinery is hijacked to modify effector proteins secreted by pathogenic Legionella pneumophila during infection to assist in invasion and survival of the pathogen. It is currently unknown whether this is a broad survival mechanism used by other pathogens during human infection. In this study, a continuous spectrofluorometric assay was used to measure the catalytic efficiency of mammalian FTase and GGTase-I with a dansylated peptide library comprised of 27 unique CaaX sequences from the C-termini of proteins from a variety of pathogens. We found that 21% of the peptides analyzed are FTase substrates and 10% of the peptides are GGTase-I substrates under multiple turnover conditions. Identifying other bacteria capable of hijacking prenyltransferases and the bacterial proteins modified during infection may assist in the development of prenyltransferase inhibitors as novel antibacterials.

References


Poster Presentation

Macaca fascicularis population structuring dictates distribution of genetic variation in Blastocystis across two islands in Southeast Asia

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Blastocystis are protozoan parasites that live in the gastrointestinal tracts of long-tailed macaques (Macaca fascicularis) and humans, among other species. Blastocystis transmission routes remain largely unknown and unstudied. Blastocystis infection in humans is known to cause severe diarrhea and gastrointestinal tract infections. Long-tailed macaques in Singapore and Bali, Indonesia, have constant contact with humans and are known to harbor Blastocystis. Our hypothesis is that the host is shaping the population structure of the parasite. By looking at the population structuring of the parasite we expect to get a better idea of the transmission route. If the parasite population structuring matches that of the host, then a fecal-oral transmission route is implicated. If these patterns do not match, then other factors must be involved. To address this question, DNA was extracted from stool samples of long-tailed macaques. DNA was amplified with subtype 3 specific primers and sequenced at 1 and 4 loci to detect variation within the subtype. Preliminary results show some sub structuring in nuclear DNA and no significant sub structuring in mitochondrial like organelle DNA. Suggesting that the population structuring of the long-tailed macaques is not directly responsible for the Blastocystis population structuring.
Experimental verification of the coupling of the Higgs Boson and the massive top quark can provide evidence for the properties of the Higgs with respect to the Standard Model. A search for Standard Model Higgs Boson production in association with a top-quark pair ($t\bar{t}=t\bar{t}H$) using an opposite-charged dilepton analysis is presented. Previous studies of $t\bar{t}=t\bar{t}H$ production have not focused on Higgs decays to opposite-charged dileptons, and findings from this analysis can provide another perspective to the understanding of the Higgs-top quark coupling. Using Boosted Decision Tree (BDT) techniques, Higgs dilepton decays were separated from Higgs decays resulting in zero or one lepton, using distinguishing characteristics of each decay signature. These two decay channels were then further separated based on number of jets in order to optimize signal sensitivity. Another BDT analysis was used to isolate all $t\bar{t}=t\bar{t}$ decays from background events. A median upper limit of 9.2 times the Standard Model expectation is expected for $t\bar{t}=t\bar{t}H$ production.
Nuclear incompressibility is the curvature of the equation of state of nuclear matter at saturation density. The preferred medium through which we quite effectively study and then constrain incompressibility is the isoscalar giant monopole resonance (ISGMR), one breathing mode of the nucleus. Using the nuclear optical model to both fit and reproduce elastic and inelastic scattering patterns, respectively, we can translate our calculations to the strength of the monopole and ultimately incompressibility. With the advent of radioactive beam facilities have come excellent experimental advancements. From here we begin to discern which probes are ideal for use in nuclear collisions. Deuterium is presently being tested for its feasibility. The Research Center for Nuclear Physics at Osaka University in Japan was home to just such an experiment. A 196 MeV $^2$H beam was impinged on $^{116}$Sn, $^{28}$Si and $^{58}$Ni targets to measure the elastic and inelastic cross-sections at various angles. These angular distributions have been analyzed using the hybrid optical model. Results of this analysis will be presented.
Semiconductors are neither an insulator nor a conductor, but can take on characteristics of both types of materials. We can control the properties of semiconductors based on the type of material we use. The most commonly used semiconductor is silicon because of its abundance, low cost, chemical stability and high quality interfaces. In Dr. Wistey’s group they are using germanium semiconductors, which can improve performance over silicon for photo-voltaic applications. By exploiting how electrons behave in germanium, photons can be absorbed more efficiently than in silicon, while retaining a comparable ability to extract electrons for energy generation. To test the quality of germanium, I assembled and fine-tuned a photo-luminescence setup, which probes the efficiency of optical processes in the material. The system is composed of a spectrometer, an infrared detector, a lock-in amplifier, beam guiding optics and a laser to excite electrons in germanium. I was responsible for aligning the optics, interfacing the software with the spectrometer and obtaining optical data from semiconductor samples. The curriculum plan is showing the students how difficult solar cells are to create. The model is a titanium dioxide-doped conducting glass with a berry dye to absorb the sunlight in the visible range. They will test their results in the classroom and then we will take the cells to Notre Dame to test their efficiency in the Kamat Lab. The students will also get a tour of the lab and have the opportunity to see research first hand.
Asymmetric, Metal-free Dihydroxylation Reaction using the Cyclic Peroxide of 1,1’-Binaphthyl-2,2’-dicarboxylic Acid

Christina Na
Advisor: Masato Koreeda, Dept. of Chemistry, University of Notre Dame

Asymmetric, metal-catalyzed dihydroxylation is one of the staples of modern synthetic reactions [Kolb, VanNieuwenhze, Sharpless Chem. Rev. 1994, 94, 2483]. In recent publications, Tomkinson’s group reported the first metal-free dihydroxylation of alkenes using malonoyl peroxides [J. Am. Chem. Soc. 2010, 132, 14409; Chem. Sci. 2014, 5, 1777]. In conjunction with our continued interest in the use of chiral 1,1’-binaphthyl systems in synthesis, we have initiated a study toward developing a new method for asymmetric dihydroxylation using the cyclic peroxide 1 of chiral 1,1’-binaphthyl-2,2’-dicarboxylic acid (2). We will present an improved synthesis of racemic dicarboxylic acid 2 from 1,1’-bi-2-naphthol (3), and the results of the use of racemic peroxide 1 in the dihydroxylation of alkenes.

\[
\begin{align*}
\text{3} & \rightarrow \text{4} + 2 \text{X} \\
\text{Pd (catalyst)} & \text{Xantphos (catalyst)} \\
\text{Toluene or DMF} & \text{90\(^\circ\)C} \\
\end{align*}
\]

\(X = \text{Phenyl or 2,4,6-trichlorophenyl}\)
A Multi-Reflection Time-of-Flight mass spectrograph (MR-TOF) is being designed for the future Notre Dame Radioactive Ion Beam facility. The MR-TOF will provide isobarically pure beams to experiments. Design considerations for the MR-TOF include its geometry, its electrode voltages, and the choice of ion extraction scheme. These considerations were investigated using SIMION simulations. As a benchmark, we first optimized the electrode voltages of the ISOLTRAP MR-TOF geometry. The preliminary simulations involved varying two electrode voltages with the remaining electrodes held fixed and resulted in a mass resolving power \( \frac{\text{TOF}}{\Delta \text{TOF}} \approx 45,000 \). Further simulations to optimize the remaining three electrodes will be required to reach higher mass resolving power.
Poster Presentation

Actin-mediated IKNM in Regenerating Adult Zebrafish Retina

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Over 39 million people worldwide suffer from blindness, while age-related macular degeneration is one of the leading causes of vision loss in the elderly. Once destroyed, human retinal tissue cannot regenerate, leaving only limited treatment options to slow disease progression. Danio rerio (zebrafish), however, have the ability to regenerate lost retinal neurons. Exposure to high intensity light, which causes photoreceptor cell death, induces zebrafish Müller glia in the inner nuclear layer (INL) to enter the cell cycle. Following completion of S-phase (approximately 35 hours after starting light treatment), nuclei migrate apically to the outer nuclear layer (ONL) where they undergo mitosis, giving rise to neuronal progenitor cells (NPCs) that further proliferate in the INL. NPCs undergo a similar migration pattern in phase with the cell cycle. This movement, termed interkinetic nuclear migration (IKNM), also occurs during retinal development, where NPC’s rapid apical movement is driven by actomyosin forces. Mechanisms governing IKNM during retinal regeneration have not been established.

To test whether the actin cytoskeleton mediates Müller glia and NPC IKNM during retinal regeneration, light-damaged adult albino zebrafish were exposed to an actin polymerization inhibitor, Cytochalasin D or its vehicle control DMSO, from 28-35 or 65-72 hours, respectively. To assess whether IKNM was disrupted, the position of mitotic nuclei was determined in retinal sections using immunocytochemistry to phospho-histone 3 (pH3, a marker for mitosis) and the nuclear dye DAPI (to label the different nuclear layers in the retina).

In DMSO control, the majority of pH3-positive cells were located in the ONL and apical INL, with few in the basal INL at 35 hrs, while Cytochalasin D caused significantly more pH3-positive Müller glia nuclei to remain in the basal INL at the expense of those migrating to the ONL. In contrast, at 72 hrs when NPC nuclei migrate, no significant difference was observed in the distribution of pH3-positive NPC nuclei between DMSO controls and Cytochalasin D-treated zebrafish. Currently, phalloidin-labelling is being conducted to visualize the potency of Cytochalasin D to block filamentous actin formation. Taken together, these data may suggest that Müller glia and NPCs use different mechanisms to drive IKNM.
Poster Presentation

Non-Boolean computing using oscillators

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Tasks of human cognition are usually mimicked as data intensive number crunching computations using modern methods. Image recognition is an example of such and has importance in areas as varied as social media to national security. The brain is able to recognize an image in what seems like no time at all yet, to compute such a task using digital logic requires much more time and expends more energy. The presented research looks to design and implement a type of neurocomputer that might mimic the oscillatory nature of neurons in the brain. It is the aim of this research to replace conventional CMOS technology with programmable nano-oscillators connections per N computational nodes thus making a usable circuit generally impractical. The paper attempts to offer a solution to this fundamental problem by coupling the oscillators in a special way. Each oscillator is connected to one-another via a communal node which itself is driven by a complex waveform whose characteristics are the basis of this research. This approach requires N connections for N computational nodes and is robust in that it does not rely on the oscillators having exact phase or frequency values for the computation to work. This neurocomputer model has shown to exhibit 3 to 4 orders of magnitude reductions in power dissipation as well as being faster than comparative CMOS computations using Boolean logic.
**Poster Presentation**

*Depositing and characterizing two-dimensional electrolytes for low-voltage memory*

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To decrease global energy consumption, low power electronic devices are needed. An example of one specific need is low-voltage flash memory for low-voltage logic devices. The aim of this project was to explore new electrolyte materials for a low-voltage memory device that involves the movement of ions within and between two-dimensional (2D) materials. The 2D electrolyte consists of a planar molecule, 15-crown-5-ether-substituted cobalt(II) phthalocyanine (CCP), doped with lithium ions and deposited on a graphene surface. The first step of the project was to deposit and characterize the CCP without ions on a graphene surface. Low concentrations of CCP (0.3 mg/L) were deposited by drop-casting in a solvent mixture of benzene and ethanol (9:1), followed by annealing at 180 °C in an argon-filled glovebox to produce monolayers of CCP on a highly ordered pyrolytic graphite (HOPG) surface. The resulting monolayers were characterized using an atomic force microscope (AFM), located in the same argon-filled glovebox. The thickness of the CCP monolayer was approximately 0.5 nm, in agreement with theory. Large numbers of nanometer-sized CCP aggregates were initially observed on the surface; however, further annealing in air reduced the size and number of particles. Because the CCP molecules are hygroscopic, we suggest that the water molecules in the air increase the mobility of the CCP, allowing the large clusters to spread out into a monolayer. Current-voltage (IV) measurements were performed on the CCP monolayer and bare HOPG using PeakForce tunneling AFM (PFTUNA). Bare HOPG produced an IV curve similar to that of a conductor, whereas the monolayer of CCP made the curve more resistive. To increase the surface coverage, the solution concentration was increased by a factor of ~40 to 13 mg/L followed by annealing in argon and air respectively at 180°C. This treatment resulted in a nearly full monolayer of coverage. Finally, in preparation for a device, ions were introduced by adding lithium perchlorate (LiClO4) to the CCP. The first deposition of CCP/LiClO4 on HOPG shows that the LiClO4 prevents the formation of a monolayer and increases the fraction of large aggregates.

![CoCRPc (CCP) molecule](image1.png)

![AFM image of CCP monolayer on HOPG](image2.png)

**Fig. 1** (a) CoCRPc (CCP) molecule - used to create 2D monolayer. (b) AFM image of CCP monolayer on HOPG. (c) Line scan of yellow line indicated in (b). Monolayer thickness = 0.5 ± 0.1 nm.
Vitamin B12, an essential molecule in many biological processes, consists of a class of vitamers known as cobalamins (Cbl). Each Cbl contains a cobalt atom centered in a Corrin ring with an upper and lower axial ligand; the lower ligand is supplied by a dimethylbenzimidazole group attached to the Corrin ring, while the upper axial ligand varies between methyl (Me), 5’-deoxyadenosyl (Ado), hydroxyl (OH), and cyano(CN). The photostability of the non-alkyl cobalamins has been widely acknowledged until recent studies showed the possible photolytic bond cleavage of hydroxocobalamin. If indeed OHCbl undergoes photolysis, the reaction could serve as an alternative source of hydroxyl radicals, which are used in the investigation of DNA and RNA structures. The purpose of my studies is to show whether or not OHCbl experiences photolytic bond cleavage and, if so, under what conditions. Ultraviolet-visible (UV-Vis) spectroscopy was utilized in conjunction with ultrafast transient absorption difference (TA) spectroscopy to report any possible photoproduct yield. The results indicate that OHCbl does not photolyze to form cob(II)alamin and hydroxyl radical after irradiation solely in the presence of radical scavengers. However, an ongoing study suggests that OHCbl may undergo photolysis in the presence of DNA. Further studies will be conducted to investigate this hypothesis and the mechanism by which the reaction proceeds.
Poster Presentation

*Development of Paper-based Electrochemical Measurements for Biosensing*

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In a normal steady state with adequate tissue resources and oxygenation, cells generate most of their cellular energy by means of the citric acid cycle and electron-transport chain, where pyruvate products from glycolysis are converted to adenosine triphosphate (ATP), a cell’s energy currency. In contrast, when under inadequate oxygen environments, cells undergo anaerobic metabolism to produce a significantly lesser amount of ATP by converting pyruvate to lactate, thus regenerating NAD$^+$ to perpetuate glycolytic ATP production. Low levels of lactate production persist even under oxygen-rich condition but below 1 mmol/L in arterial and venous blood. In sepsis patients, however, level of lactate are significantly higher due to strained cellular metabolism in major tissues and muscle cells. In this study, we describe a method for determining lactate concentrations by using a low-cost, paper-based, electrochemical device (PED). The device was fabricated using pencil-drawn carbon electrodes and wax-patterning technique to secure sample placement. The device was characterized through cyclic voltammetry and differential pulse voltammetry of potassium ferricyanide. Various electrode configurations were investigated such as the difference in electrochemical response between drawn counter electrode (CE) and reference electrode (RE) versus using a traditional CE and RE. The development of a paper-based electrode results represents an important step in creating a low cost, paper-based electrochemical biosensor for low resource environments.
**Poster Presentation**

*Discovery and Validation of a Y-locus in Aedes aegypti and Determination of Polyandry*

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Diane Lovin  
David Severson  
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*Aedes aegypti* is the primary vector of the viruses that cause dengue, yellow fever and Chikungunya. In the past half century, prevalence of dengue fever has drastically emerged with a current estimate of 50 to 100 million individuals infected yearly. The absence of available vaccines requires that vector populations be reduced in order to combat outbreaks. Past techniques used to suppress mosquito populations have generally not shown lasting effects. Therefore, interest in genetically modified mosquitoes has arisen through techniques such as the sterile insect technique (SIT) in males. However, in order to have a successful cycle of genetically modified *Aedes aegypti*, the details of the mosquito’s behaviors must be identified, in particular the sexual behaviors. It has generally been assumed that female *Aedes aegypti* are monandrous, meaning that females only mate with one male. Conversely, studies have suggested that possible polyandry is present (Helinski et al. 2012). However, multiple male sperm in the female spermathecae has not been yet identified by the usage of the male Y-locus to determine polyandry. This is due to a lack of a known Y-locus in the male *Aedes aegypti* genome. Primers were designed in search of the Y-locus and run through PCR in search of male only amplification. As of now, we have not discovered the Y-locus. The possible presence of polyandry was subsequently investigated through spermathecae dissection and genotypic analysis.
Filaments are tube-like structures filled with matter and gas that give the universe a web-like appearance. In order to study the significance of these large scale structures, numerous structure finding algorithms have been created in order to detect tubes in computational models. The aim of this paper is to determine the mathematical underpinnings of a few select structure finding algorithms and understand which parts of the filament these algorithms are recreating. This was done by selecting three astronomical structure finding algorithms and one medical imaging algorithm. The equations and their spatial significance were compared in order to understand what these algorithms offer. It was determined that in order to ensure proper tracing of the filaments, centerline extraction used in medical imaging would provide better data. Using python, the equation used for centerline extraction was written in a way that it could attempt to be adapted to astronomical computations. Furthermore, incorporating other features of the physical attributes of filaments such as Gibbs Free Energy would allow more significant study of the nature of such large scale structures. For future work, Gibbs Free Energy could be determined based on the initial data and then compared to the structure finding algorithm.
Poster Presentation

Production and Purification of P.69T 2K for mimicking its secretion through its own translocator domain

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Benjamin Cressiot
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Autotransporters are the largest family of virulence proteins secreted from Gram-negative bacteria. We use pertactin as a model autotransporter from Bordetella pertussis to study its secretion through its own translocator domain. It is not clear how pertactin is secreted through the outer membrane efficiently without assistance from an external energy source such as ATP or a proton gradient. A vectorial folding mechanism of the passenger has been proposed to drive pertactin secretion to the outer membrane1. In order to understand how autotransporters are secreted through their own translocator domain, we purified pertactin-2K to mimic the secretion using an electrophysiological method2 at the single molecule level. We produced by recombinant methods pertactin-2K, which forms cytoplasmic inclusion bodies in E. coli. The inclusion bodies were solubilized and the proteins were refolded by stepwise dilution and dialysis. We then purified the protein on an anionic exchange column and an exclusion size column. Finally, we checked the unfolding properties of pertactin-2K by tryptophan fluorescence.

Poster Presentation

The role of Scribble in epithelial cancer metastasis

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Previous studies have revealed the importance of epithelial-mesenchymal transition (EMT) in the conversion of benign tumors to invasive and aggressive cancers in epithelial cells. Integral in normal development, during cancer progression EMT enables cancerous cells in primary tumors to lose their polarity and cell-cell adhesions, break through the basal lamina, and enter the bloodstream. This transition is especially relevant because of the importance of stopping cancerous growth before metastasis, when it is much more difficult to treat and eradicate. Interestingly, EMT corresponds with the protein Scribble (Scrib) becoming mislocalized within the cell. In healthy human epithelial cells, Scrib is normally localized at the cell membrane, where it plays a role in maintaining cell polarity. We hypothesized that Scrib’s localization at the membrane may be promoted through palmitoylation, a post-translational modification that attaches fatty acids to the protein. The mislocalization of Scrib within the cytosol, instead of the membrane, has been shown to be associated with increased metastatic spread of cancers. Genetic knockdowns of Scrib have suggested its role as an important tumor suppressor and further studies into the regulation of Scrib in cancerous cells have resulted in interest in the in vivo thioesterases APT1 and APT2 and their key role in Scrib palmitoylation turnover. Cells overexpressing APT1 and APT2 exhibit phenotypes of EMT cells, with Scrib localized in the cytosol. We have previously seen that specific inhibition of APT2 restores Scrib’s membrane localization in EMT cells. Our research explores the mechanism of APT2 and Scribble interaction and we are specifically interested in the potential roles that Scrib’s domains may play in regulating cell polarity and EMT.
Poster Presentation

*Speciation of Organic Compounds in Cloud Water from Whiteface Mountain*

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Julia Laskin  
Alexander Laskin  
James Dukett  
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Clouds play an important role in the Earth’s climate through active participation in the hydrological cycle (precipitation) and by affecting the total albedo of the planet. The cloud formation process, in which supersaturated water condenses onto particles, results in an unique aqueous chemical environment within cloud droplets. Very few studies have examined high molecular weight organic compounds present in cloud water. These soluble organic compounds in cloud water are hypothesized to comprise a significant mass fraction of atmospheric aerosols upon cloud droplet evaporation. To study the organic composition of cloud water, samples were collected at Whiteface Mountain in New York from September 25-27 2013. A LTQ-Orbitrap mass spectrometer with electrospray ionization was used for high resolution mass spectrometry analysis, which provides detailed molecular characterization. NOAA HYSPLIT backward air mass trajectory analysis was performed to determine the source regions of the particles impacting the cloud water. Google Earth was used to overlay trajectories with a MODIS satellite fire detection map to check whether smoke affected the chemistry of the cloud water. Relationships between organic and inorganic compounds were analyzed through comparisons of the concentrations of total organic carbon and inorganic ions with pH and organic compound classes, as determined by mass spectrometry. To examine the structures of several organic ions, tandem mass spectrometry analysis was conducted to determine mass losses upon fragmentation. Overall, understanding the organic composition of cloud water can help determine the chemical processes that occur in clouds.
Artificial Tissue Formation Using Laser-Based Optical Tweezers

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Koshala Sarveswaran
Volker Kurz
Zhuxin Dong

Advisors: Tetsuya Tanaka, Dept. of Chemical and Biomolecular Engineering and Gregory Timp, Dept. of Biological Sciences and Electrical Engineering, University of Notre Dame

Synthetic capillaries are essential for further advancements in the field of tissue engineering. The ability to mimic in vivo human capillaries would serve a variety of purposes for medical advancements. Without mastering engineered capillaries, larger structures are impossible to maintain due to hypoxic stress and necrosis.1-7 Here, it is shown through “live cell lightography” that it is possible to develop a tissue that mimics a capillary in an in vitro environment. Using time-shared optical tweezers, cells can be easily manipulated in a microfluidic device to a desired three dimensional position. In order to fix the cells in place, the cells are suspended in a mixture of photo-polymerizable hydrogels that can be activated under exposure to ultraviolet light. To ensure that these capillaries truly represent in vivo tissue environments, measurements were taken on both the capillary and the hydrogel surrounding for comparison. It has been found that several similarities exist between true capillaries and their synthetic counterparts. The hydrogels have similar porosity and elastic properties to the extra-cellular matrix, which encapsulates true human tissues. Also, the velocity and wall shear stress of red blood cells traveling through varying lumen areas expresses similar trends to research on in vivo capillaries. These tissues can serve a variety of purposes. One effective application of our capillaries would be seen in metastasis studies. In the future, we plan on adding cancer cells along with red blood cells. If our capillaries behave similar to in vivo tissue, we should observe the red blood cells avoid endothelials but the cancer cells burrowing into the endothelial wall, through pericytes and fibroblasts and exit to the surrounding. Quantifiable data such as average metastasis time and percentage of cells that metastasize could be measured and used for diagnostic tools. In a similar manner, our capillaries could be used to study drug delivery through the blood stream and even diseases such as systemic capillary leak syndrome (SCLS) without having to do in vivo testing.
Poster Presentation

Classification of divalent cation effects on motility patterns of the bacterium Pseudomonas aeruginosa

Sarah Philo
Advisor: Joshua Shrout, Dept. of Biological Sciences and Civil Engineering and Geological Sciences, University of Notre Dame

Pseudomonas aeruginosa is a ubiquitous bacterium and is recognized as an opportunistic pathogen that causes a variety of diseases in immunocompromised individuals. For example, P. aeruginosa infections are generally acute in burn wounds and the eye and chronic in the lungs of individuals with Cystic Fibrosis (CF). The dense anaerobic biofilm of P. aeruginosa in the CF lung renders many antibiotic regimens unsuccessful. While these various infections are known to occur, little is understood about how P. aeruginosa senses its surrounding environment during its transition to cause infection in a human. Further understanding the environmental role in its growth may allow for prevention and/or improved treatment of these infections. It is also important to understand motility of these bacteria to fully characterize the course of entry into the host and subsequent infection. The elements calcium and magnesium are required in trace amounts for P. aeruginosa growth and have been shown to affect P. aeruginosa biofilm structure and attachment, but less is known about how Ca and Mg influence P. aeruginosa motility. In general, wild type P. aeruginosa are motile and are capable of swimming, swarming, and twitching using flagellum and type IV pili (TFP). In this study, motility patterns of P. aeruginosa strains CF39 and MH340 are observed under extreme calcium and magnesium conditions. It was shown that both divalent cations are needed for swarming motility and that excess calcium and limited magnesium reduce swarming. MH340 twitching is reduced in conditions with both limited and excess calcium. Results suggest dependence on environmental cues for proper flagella and TFP function. Future studies aim at observing the phenotypes of MH340 and CF39 in anaerobic conditions with varying ion concentrations, as well as creating a gain-of-function CF39 twitching mutant.
Two hundred eighty-five million people worldwide are visually impaired, and many exhibit a progressive and irreversible vision loss. If it were possible to regenerate the damaged/lost retinal neurons, their vision could be restored. In contrast, zebrafish can regenerate all their retinal cell types, making it an ideal organism to study neuronal regeneration and elucidate the mechanisms that could restore sight to the visually impaired. Zebrafish rod precursor cells, which arise from proliferating Müller glia, are required for the persistent production of rod photoreceptors throughout the life of the fish. It was previously described that rod precursor cells increase their rate of proliferation in response to light-induced rod photoreceptor death. We examined rod precursor cell proliferation and demonstrate that there is no significant difference in the number of proliferating rod precursor cells in both undamaged and light-damaged retinas that were dark-adapted. However, undamaged dark-adapted fish possess significantly greater numbers of proliferating rod precursor cells relative to fish that are maintained in standard light conditions. These data suggest that prolonged dark adaptation induces rod precursor proliferation rather than light-induced rod photoreceptor cell death. To determine the onset and contribution of Müller glia proliferation to the increased dark-adapted rod precursor proliferation response, we are carrying out a detailed timecourse analysis (0, 2, 5, 8, 11, and 14 days) using Tg[gfap:EGFP] zebrafish, which express EGFP specifically in Müller glia. In addition, we are testing the possibility that increased cell death causes elevated rod precursor cell proliferation during dark adaptation using the TUNEL assay.
Hydrogen Production from Ammonia-Borane using Ruthenium as a catalyst

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Haitao Wang
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Advisor: Chongzheng Na, Dept. of Civil Engineering and Geological Sciences, University of Notre Dame

Hydrogen is commonly regarded as the simplest and most abundant element in the universe. The scientific community estimates that 90% of our visible universe is composed of hydrogen. Ammonia Borane is a chemical compound which is approximately 20% hydrogen by weight, having the chemical formula NH3 BH3. This colorless solid is a simple boron-nitrogen-hydride compound and has attracted a lot of attention as a source of hydrogen fuel. However, a catalyst is required for the hydrolysis generation of hydrogen (H) gas from the NH3BH3. The highest active catalyst being examined for testing is Ruthenium (Ru). When extracting H2 from the readily available source such as freshwater (H2O), an energy source from an electrical charge is required, whether it be generated from a turbine or collected from solar support. This process is called “on board” and tends to logistically create space and weight issues for the mode of transportation. Ru, when used as a catalyst, generates H2 (gas) at room temperatures from NH3BH3. The purpose of this investigation is to effectively produce H2 gas from NH3BH3 at room temperatures without additional energy input. In turn, by using the chemical compound we will be eliminating the need for additional electrical input for extracting/producing H and freeing-up gravimetric mass and volumetric space.
Autism Spectrum Disorder (ASD) is a neurodevelopmental disorder marked by impaired social interaction/communication along with stereotyped/repetitive play. There is a pressing need for interventions that increase social interactions with typically developing (TD) peers. The goal of this study is to evaluate whether a shared interest in robotics was more prevalent in conversations between autism spectrum disorder (ASD) adolescents and typically developing (TD) peers after a weeklong robotics summer camp. Eight individuals with ASD and eight TD peers ages 12–17 participated in a weeklong robotics camp, during which they learned robotic facts, actively programmed an interactive robot, and learned “career” skills. Before and after camp, each pair of participants was asked to interact for 10 minutes. The room had several robot-related items along with other games, toys, magazines, and snacks. They were instructed to get to know each other. We evaluated pre- and post- camp interaction sessions and calculated: the number of times the word “robotics” or “robots” was said between the participants as they conversed with one another, and the number of times the two participants interacted with any of the robotics items in the room. Participants with ASD had a small increase from pre- to post- in the number of social interactions in which robotics was the shared topic of their conversation. Our findings suggest that a summer robotics camp encouraged ASD participants to have more social interactions in which robotics was the topic of their conversation. Moreover, TD participants experienced an increase in the number of occurrences where participants played with the robotics items in the room. Furthermore, our findings suggest that a summer robotics camp increased TD participants’ interest in robotics.
As robotic technology advances, autonomous robots will be increasingly used for a variety of functions in human-social environments (HSEs) [1]. In order to effectively serve their purposes and integrate, robots in human-robot interaction (HRI) situations must be able to understand and respond to high-level social signals. For example, a robot should perceive a person's raised hand as a signal to stop, and consequently discontinue its task. However, computationally determining these social signals and developing responses remains a challenge in HRI [2].

In some HSEs, coordinated joint action of groups naturally exists as a social signal or may even be necessary for accomplishing a task [2]. For example, pairs rocking in chairs unintentionally exhibit synchrony in their rocking frequencies when instructed to rock at a comfortable rate [3]. Dancers executing choreographed routines move with steps that are either complementary to one another or identical. Because of the presence of joint action in HSEs, robots need to be able to recognize it and participate appropriately. We previously proposed an event-based method for measuring the degree of synchrony of a group, and demonstrated the method's ability to accurately determine synchronous and asynchronous conditions [4-5]. However, extending the event-based method to analyze data collected on multiple systems from new Kinect sensors requires a system for time-synchronized collection of the sensors' data streams. The multimodal Kinect for Windows sensors provide RGB, depth, skeletal, and audio data, which enable the analysis of joint action.

To facilitate the study of joint action with this new technology, we developed software components that implement a Client-Server architecture for recording Kinect data. The server sends commands to client nodes instructing them to synchronize their system times with that of the server, start recording, and stop recording. The clients, upon receiving the commands, automate the Kinect Studio tool using Windows UI Automation to establish an optimal recording environment and control the interface of the tool. This system will enable expanded opportunities for analyzing joint action using the improved technology of Kinect for Windows sensors and multiple vantage points for recording.

Flavodiiron nitric oxide reductases (FNORs) are enzymes that catalyze the reduction of nitric oxide (NO) to N2O in pathogenic bacteria. Nitric oxide is used by the body for signaling and in the immune system in fighting bacterial infection. Hence, the detoxification of NO by certain pathogenic bacteria is of interest to the fields of bioinorganic chemistry and immunology, as this provides resistance to the pathogens against NO and allows them to more easily infect the human body. However, the mechanism of NO reduction by FNORs is not known. Previously, our group reported that the FNOR model complex [Fe2(BPMP)(OPr)(NO)2](BPh4)2 rapidly produces N2O upon two-electron reduction. In order to further explore the chemistry of this complex, we have synthesized the water-soluble analog [Fe2(BPMP)(OPr)(NO)2](OTf)2. By changing the counterions of the model complex from tetraphenylborate to triflate anions, the solubility in water greatly improved. The close proximity of the two NO molecules allow for nitrogen coupling and evolution of N2O upon reduction. Here, we present spectroscopic characterization of this complex as well as electrochemical characterization and reactivity in aqueous solution.
Mod5 is a yeast enzyme that plays roles in diverse cellular processes, including the modification of tRNA in the cytoplasm and targeted gene silencing in the nucleus. Mod5 displays amyloid-like biophysical properties that can confer resistance to certain antifungal agents, though it was not previously clear whether the nuclear or cytoplasmic functions were affected by the amyloid aggregation. The human homologue of Mod5, TRIT1, carries out the same tRNA-modifying action and nuclear transcription function, but it is not known to what extent the prion-like amyloid misfolding of the protein is conserved. Research into Mod5 and TRIT1 could shed light on little-understood processes, such as adaptive amyloid-like protein aggregation and spatially controlled gene silencing. Finding conservation of these roles in TRIT1 could extend the findings’ to human systems, where recent work has characterized TRIT1 as a tumor suppressor.

Part of the project has focused on interactions between different functions of Mod5. For instance, antifungal treatment to select for aggregated Mod5 phenotypes was followed by testing for the effects on nuclear silencing activity, supporting the hypothesis that cytoplasmic and nuclear roles of Mod5 appear to operate independently. Another arm of research involves production and purification of Mod5 and TRIT1 proteins for in-vitro assessment of biophysical properties of the proteins. These experiments on the purified proteins are in progress.
Poster Presentation

*Material characterisation of hybrid organic/inorganic perovskites for solar cell applications*

Barry Reid  
Joseph Manser  
Advisor: Prashant Kamat, Dept. of Chemistry and Biochemistry, University of Notre Dame

Perovskites are the general name given to compounds with a formula of AMX₃ whereby A and M are cationic atoms and X is an anionic constituent. The atoms combine to form an octahedral network which were identified as potentially useful due to their conductivity and photoactivity. Recently there has been growing interest in inorganic/organic hybrid perovskites consisting of an organic cation in the A position, divalent metal cation (M) and a halogen (X) to form three dimensional structures. These hybrid perovskites combine the attributes of the organic and inorganic components and have been identified for use as light harvesters in solar cells as the large band gap allows strong broadband absorption of solar energy. In this poster(presentation?), the crystallographic and thermal properties of lead and tin halide perovskites are investigated with the aim of determining the effect of different preparation methods on the properties of the final perovskite material. The characterisation is carried out using X-ray diffraction (XRD) and thermogravimetric analysis (TGA). The results show that the hybrid lead perovskites exhibit differing X-ray diffraction peaks when prepared using mechanical activation compared to spin-coating methods. Variation in the molar ratio of the precursor components (CH₃NH₃I/PbI₂) leads to differences in the character of spin coated films. Tin-based hybrid perovskites were found to decompose at lower temperatures than the lead based equivalent.
Poster Presentation

ULTRAFAST OPTICAL INVESTIGATIONS OF DIPOLAR AND QUADRUPOLAR MOLECULES OF THIOPHEN-2-YL PYRIDINIUM IODIDES WITH VINYL LINKAGES

Federica Ricci
Oluwasegun Adegoke
Advisor: Theodore Goodson III, Dept. of Chemistry, University of Michigan

Emerging technologies in biology, medicine, optics and imaging, are in continuous need for new, high-performance and low cost materials. There has been intense study of the dipolar compounds of electron donor (D) and electron acceptor (A) groups with π-linkage for their nonlinear optical properties in the past decades. However, the photophysical properties of the more promising complex quadrupolar systems (D-π-A-π-D or A-π-D-π-A) still need to be deeply understood and modeled. Methyl pyridinium salts fall into this group of compounds with potential applications in the medical and optoelectronic fields due to their nonlinear properties and ability to form complexes with DNA. In this study, two trans 2-(thiophen-2-yl) vinyl pyridinium iodides, C1 and C2, were studied by ultrafast spectroscopic techniques. The dipolar C1 has an acceptor unit of methyl pyridinium linked to a donor unit of bithiophene (D-π-A) with a dialkylamino substituent in the alpha position of the terminal thiophene ring. On the other hand, the quadrupolar C2 had an additional donor unit of bithiophene attached to the acceptor unit of methyl pyridinium, thereby forming a D-π-A-π-D configuration. C2 is symmetrical about the methyl pyridinium unit. The effect of the surrounding media on the photophysical behaviors of the compounds were investigated by measuring their steady state properties in solvents of different polarities. The lifetimes of the compounds were measured by using the femtosecond time-resolved up-conversion technique. The lifetimes of C1 and C2 were found to be 4.77 ps and 0.48 ps respectively. The two-photon absorption cross-sections of the samples were also measured through two-photon excited fluorescence method (TPEF). This study demonstrates the enhancement in the nonlinear properties of the quadrupolar compound over its dipolar counterparts.

REFERENCE


An ongoing research collaboration focuses on developing Paper Analytical Devices (PADs) to test for substandard pharmaceuticals. Part of this process involves the colorimetric analysis of chemical reactions that take place on the PADs, that determine the quality of the pharmaceutical. The developed computational analysis software locates the regions of interest and is used to catalog data corresponding to colors detected. The software can also compare unknown PAD samples with the cataloged data of known samples. This process removes human obstacles of qualitative determination and provides qualitative results.
Poster Presentation

*Development of novel organometallic catalysts for the copolymerization of carbon dioxide and epoxides*

Arianis Riofrío Díaz  
Jeremy Eberle  
Advisor: Kenneth Henderson, Dept. of Chemistry and Biochemistry, University of Notre Dame

Since carbon dioxide (CO$_2$) is a nontoxic, abundant, and biorenewable resource, its transformation into useful products is a topic of interest. Among the possibilities, polycarbonates can be produced from the copolymerization of CO$_2$ with epoxides, which is a greener alternative to otherwise toxic synthetic pathways. For that reaction the rate-determining step is the epoxide ring opening; that is why developing catalysts that can help relieve the ring strain is of great importance if this new kind of approach is wanted to be taken to industrial levels. During the 2014 summer nine new mononuclear organometallic complexes were developed utilizing zinc, magnesium and aluminum. The ligand set used for that purpose was based on salicylaldimine derivatives from the Schiff base condensation of a salicylaldehyde derivative and a diamine. Currently the catalysts’ ring opening capacity is being studied by conversion via gas chromatography and NMR.
Raman spectroscopy is a useful analytical tool for biomolecular characterization. Differences in the structure of glycans, or carbohydrates in the human body, correlate to distinct functions, necessitating accurate identification. Isomeric structures of carbohydrates are difficult to identify by many methods; however, Raman spectra provide distinct spectra associated with subtle changes in chemical structure. The Raman effect is weak as only 1 out of $10^{13}$ photons Raman scatter, so surface-enhanced Raman spectroscopy was developed as a way to increase signal in order to collect more chemical specific information. SERS uses metal nanostructures, which are irradiated with a laser at their plasmon resonance frequency, resulting in enhancements of up to $10^{13}$ in the Raman scattering of the molecules of interest on the surface. Even though this method has advantages over Raman scattering, there are still drawbacks, as nanostructures only interact with molecules that are within a few nanometers of the surface, and it can be difficult to obtain reproducible signals using SERS. Recent work in the Schultz lab has led to the development of a flow cell which uses a sheath flow to force the analyte close to the surface of the nanostructures, leading to increased sensitivity and reproducible signals when working with analytes in solution. This summer, work has been done to show that simple sugars acting as model carbohydrates can be detected using the flow cell, both with a normal SERS substrate and with SERS substrates functionalized using a self-assembled monolayer of decanethiol and mercaptohexanol. The end goal of this project is to identify specific glycans based on their Raman spectrum by using the developed SERS flow detector.
We wish to model the evolution of the feedback materials from a galaxy moving in a filament. An accurate model can be obtained by inputting the galaxy’s parameters and solving the compressible Navier-Stokes equations using a numerical solver that uses a fractional step method. Because there is material flowing in and out of the galaxy, this solver can tell us where the material is flowing to and if the orientation of the galaxy will have an effect on other galaxies or on the distribution of material in the filaments.
Because about 40% of America’s energy is consumed in building operations, great care must be taken by architects and engineers to design in an informed and responsible manner. The vast majority of design is now undertaken with the aid of computers and so it is imperative that architects and engineers be armed with competent software tools for analyzing the potential environmental impact of proposed buildings. Unfortunately, the reality of the situation is that tools of this nature available today are quite rudimentary. A quality energy analysis tool should include several key features, and all currently available tools are missing at least one of the following critical attributes; the tool should be reliably accurate and precise, should react dynamically and be usable during the design process, should make a holistic assessment of impact, and last but not least, it should be user-friendly. Here at the Green Scale Project our own new tool is in its testing phases, but in parallel with tool development time has been devoted to the analysis of case studies using several of the most popular environmental impact tools available. This comparative study is revealing the strengths and weaknesses of these commonplace tools and shows examples of the numerical variance between each of their respective outputs under a controlled experimental situation. Both the discrepancies discovered between these existing applications and the inherent weaknesses identified in this study support the need for a new tool. The particular attributes being written into the code of the Green Scale Tool respond to the shortcomings found in existing applications and should give designers a chance to practice in a more conscientious manner with far more confidence and far less effort. Providing this capability to architects everywhere has the potential to fundamentally shift the industry towards adopting more sustainable practices as habit, thereby paring down what is now an enormous sector of the planet’s energy consumption. In this way, humanity can become better, more caring stewards of what is now its only home.
Poster Presentation

*Development of novel organometallic catalysts for the copolymerization of carbon dioxide and epoxides*

Ann Rutherford
Jeremy Eberle
Advisor: Kenneth Henderson, Dept. of Chemistry and Biochemistry, University of Notre Dame

In keeping with the RET theme of Engineering a More Sustainable Energy Future, Dr. Henderson’s group is working on a project to create catalysts that promote co-polymerization of carbon dioxide (CO2) with epoxides to produce polycarbonates. These polycarbonates are higher-value polymers with applications in many areas (i.e. lightweight, shatterproof lenses) and could potentially provide a cost offset to carbon capture and sequestration efforts. Also, most polycarbonates are synthesized using phosgene, which is highly toxic, and bis-phenol-A, which is derived from petroleum. Current metal based catalyst systems utilize expensive, toxic and highly colored metals (e.g. Cr, Pt, Co). These catalysts have shown high activity for the copolymerization of epoxides with carbon dioxide. The group tries to replace those toxic and expensive metals with more active, lighter elements (i.e. Mg, Ca, Al, Zn) because these metals are more abundant, biocompatible and environmentally benign. After synthesizing several metal complexes with two different ligands, we attempted to open the epoxide ring of cyclohexene oxide using the various organometallic complexes.
Poster Presentation

Windows Azure as a Platform for Malaria Modeling

Natalie Sanders
Advisor: Alexander Vyushkov, Center for Research Computing, University of Notre Dame

Though malaria is both treatable and preventable, it remains one of the deadliest diseases on the Earth. Reducing malaria burden is a public health priority in many countries, and in silico modeling is an effective tool for developing global strategy for eradicating malaria. Using a platform of mathematical models, the risks of the disease’s transmission are interpreted with respect to ecology and vector behavior. The results of the model relate the effectiveness of malaria control tools by geographic location. While providing scientists with valuable results, such models may take several hours to complete. Consequently, the simulation runs the risk of terminating if the user’s machine is shut down, thus losing all results. By implementing the transmission models in the cloud, users may deploy several simulations at once, retrieving the results when convenient and may avoid the task of running their personal machines for the entire execution period. Windows Azure is a cloud computing platform provided by Microsoft, offering a wide array of services, including storage and backup; computing and networking capabilities; web and mobile development tools; and data and analytics processing. Utilizing Azure’s BLOB storage and computing power, we developed two Python scripts to execute the transmission models in the cloud using the Azure SDK for Python. The first script, also referred to as the host script, is run on the user’s local machine, allowing the user to run simulations on virtual machines and retrieve the results. The various simulation models are executed by using different OS images to create VMs. Each image runs a variation of another script, referred to as the VM script, which executes a specific model with uploaded inputs and returns the results to the cloud. Currently, these scripts run on Windows OS. However, it is possible for the code to be adapted for different operating systems.
Poster Presentation

Stochastic computing and nanomagnet logic (NML)

Katherine Sanders
Advisors: X. Sharon Hu and Michael Niemier, Dept. of Computer Science and Engineering, University of Notre Dame

Nanomagnetic logic (NML) is a quickly growing area of nanotechnological research. Its unique characteristics make it a strong contender for replacing present computing technology in certain applications. NML is non-volatile (retaining information without power), radiation hard (making them ideal for harsher environments), and use much less power than charge-based devices. While there are some drawbacks, using stochastic computing (SC) allows us to address these challenges. Leveraging SC computing paradigm and NML devices, we are working to create a counter. Starting with an adder of five bistable magnets from an existing work we change different parameters to allow for correct logical computation. Using micromagnetic simulation tools, simulations are run to compare the effect these parameters have on different logic cases and on the adder as a whole (based on the clocking margins), test different NML structures, and use the results to create a functional counter.
The Sahel Region in Africa is composed of Mauritania, Senegal, Mali, Burkina Faso, Chad, Niger and Sudan. It is affected by a harsh climate, religious extremism and sectarian violence. Countries such as Mali suffer from both ethnic tensions and the presence of al-Qaeda in the Islamic Mahgreb (AQIM). At the same time, Senegal has a similar history and geography, and when faced with ethnic violence, have been able to reach accords and avoid further escalation. The purpose of this study is to analyze the different conflicts, how they repeat throughout the region or how they are different, like the case of Senegal and Mali. The Sahel Region is geographically defined as the zone where the Sahara Desert transitions into the Savanna. Territorial disputes are commonly seen over the fertile Savanna, since they rely on agriculture to survive, or the petroleum-rich desert like Sudan and South Sudan. The overpopulation, the droughts, extreme poverty, human rights violations and poor central governments add to the growing tension in Mauritania and Burkina Faso. In countries like Chad, all of these factors lead to ethnic violence. Not being able to express religious or ethnic identity cultivates the resentment that leads to sectarian violence. An in-depth study of the historical background of each country was researched, working with theories that focused on internal conflict, as well as various causes of war. Stronger governments need to be built in the region, diversifying their economies to include exports in order to construct functioning infrastructure that will make access to water and food easier. It’s not until these communities reach a general better standard of living, that the conflicts be addressed. Once living conditions improve, conversations between government and rebels can begin.
Poster Presentation

Mobile Device Network Traffic Capture and Analysis

Siddharth Saraph
Timothy Wright
Advisor: Timothy Wright, Dept. of Computer Science and Engineering, University of Notre Dame

Mobile devices with Internet-access capabilities have become increasingly popular over the last few years with users often carrying them and interacting with them for much of the day. Therefore, it has become important to understand and characterize mobile device network traffic to help determine what information mobile devices are transmitting and to whom. To begin with, we study the network traffic of “inert” devices, or devices with no user input or interaction. Specifically, in this experiment, which was run twice on different days, an iPad mini (an iOS device) and a Samsung Galaxy 8 (an Android device) were given similar, minimal configurations out-of-the-box, updated, and left to sit unused for a 25-hour period. All network traffic transmitted to and from the devices during this period was redirected through a transparent proxy server. At the proxy, data were captured, processed, and stored in a database. We aim to analyze these data to determine with whom these devices are communicating, how much and how often they are communicating, what data they are transmitting and receiving, and whether there are any privacy risks while in this apparently “inert” state. We also aim to identify and explain any interesting patterns in the data and differences between the experiments.
Oral Presentation

*Analysis of schematic one-level and two-level nuclear shell models*

Jason Saroni  
Advisor: Mark Caprio, Dept. of Physics, University of Notre Dame

In the nuclear shell model, nuclei with several nucleons outside closed major shells have a prominent short-range residual interaction which can approximately be accounted for through pairing forces and deformation-inducing quadrupole forces. Here these forces are considered in a valence space of one and two shells. The calculated results are compared to test cases using the ArbModel code. The ultimate goal is to map out the competition between the pairing and quadrupole forces.
Computational schemes which provide numerical solutions to partial differential equations have myriad uses in the realm of physics and beyond, from electrodynamics to analytical finance. One of the primary limitations of high-resolution schemes is the speed and efficiency with which the model can be executed. This project sought to explore the use of a Graphics Processing Unit (GPU) to accelerate code which models three-dimensional hydrodynamic shocks. The primary advantage of utilizing a GPU over the more traditional CPU for compute-intensive numerical simulations is the presence of a much larger number of cores. In this case, the GPU used was the NVIDIA Titan Black, which contains 2880 cores. The code used was previously written by Prof. Balsara in Fortran and the acceleration directives were in OpenACC, a recently developed language for expressing high-level parallelism. This implementation intends to demonstrate the potential of GPU acceleration as a viable alternative to more costly multi-CPU systems.
The activation and oxidation of C-H bonds offers the opportunity to take advantage of functional groups that were previously ignored due to their apparent lack of reactivity. The active field of C-H activation has shown that it is, in fact, possible to transform relatively inert C-H bonds into new C-O bonds with useful and desirable functional properties. The ability to transform C-H bonds into reactive centers is especially beneficial to the area of natural product synthesis, where these new methods allow for alternative synthetic routes when traditional methods are ineffective. These unique transformations offer novel pathways towards the synthesis of complex molecules, as previously ignored portions of the molecules can now be utilized when developing a synthetic strategy. This methodology study focuses on reaction conditions to optimize the directed oxidation of a key C-H bond in a precursor to a common intermediate of a class of anti-inflammatory natural products. The strategies that are being investigated rely upon the use of a directing group for C-H activation and are first being explored in model systems before subjecting the synthetic precursor to the conditions. These strategies investigate the effectiveness of C-H oxidation using iron catalysts and conditions previously established by the White group, as well as Suarez iodination followed by oxidation.
Approximately 30% of all breast cancers involve the overexpression of ErbB2, which can promote cell proliferation and oppose apoptosis. Currently, the best treatment option for ErbB2 positive breast cancers is the drug Herceptin. But while Herceptin has shown promise, patients are known to eventually develop resistance to the drug, leading to the need to implement alternative methods of treatment. One example of alternative treatments that are being investigated to overcome these shortcomings are immunotoxins. Immunotoxins are composed of a targeting ligand and a toxin, allowing for the selective destruction of cancer cells. Here we attempt to develop an immunotoxin that will specifically target cells overexpressing ErbB2. In addition, because the immunotoxins we are interested in exert their cytotoxic effect at the cell and do not require internalization, cells will have a more challenging time becoming resistant to it. First, cells overexpressing ErbB2 were treated with a variety of peptides derived from bacteriocins and, utilizing an ethidium homodimer assay, cell death was assessed. We determined that the peptide NL11-PSA, composed of an ErbB2 targeting ligand (NL11) and a toxin derived from pardaxin (PSA), showed the strongest toxicity and specificity of all the peptides tested. In addition to screening these peptides, we have attempted to produce an immunotoxin composed of a targeting ligand and the toxin recombinantly. In tandem, these approaches represent a multi-faceted approach to target ErbB2 and our data suggests that NL11-PSA could be used as an effective therapeutic to eliminate ErbB2 positive breast cancer cells.
Oral and Poster Presentation

Blinded by the Light: A Vitamin B$_{12}$ Kinetics and Quantum Yield Study

Abigail Shepard
Daniel Ocasio
Advisor: Roseanne Sension, Dept. of Chemistry, University of Michigan

Alkyl cobalamins are a widely studied branch of vitamin B12 compounds known to be photoactive. Non-alkyl cobalamins, such as hydroxocobalamin and cyanocobalamin, are presumed to be photostable. However, hydroxocobalamin, if photochemically active, has the ability to generate hydroxyl radicals by the following reaction: OHCbl + hv yields hydroxyl radicals plus cob(II)alamin. These radicals have been proposed for use in determining the structural patterns of DNA and RNA in hydroxylation studies. The intention of our study is to provide further insight into the photostability of hydroxocobalamin. Photolysis was monitored using an Ultraviolet-Visible (UV-Vis) Spectrometer in combination with Transient Absorption Difference (TA) Spectroscopy. The purpose of this study is to determine the kinetics of the homolytic cleavage of the axial hydroxyl bond within hydroxocobalamin. The results indicate that hydroxocobalamin is unable to undergo photolysis to form hydroxyl radicals and cob(II)alamin (Cob (II)) in the presence of sodium benzoate, a radical scavenger. Future studies will be performed to investigate hydroxocobalamin’s ability to photolyze in the presence of DNA.
The electromagnetic waves in the terahertz (THz) region (0.1-10 THz) have become increasingly important for a wide range of applications including package inspection, quality control, security screening, defense, medical imaging and diagnostics, non-destructive evaluation and spectroscopic characterization of materials. Recent advancements in development of compact THz sources and sensitive detectors have paved the way for research in advanced quasi-optical THz components such as tunable filters, re-configurable lenses and mirrors for actively manipulating THz beams and radiation. The conventional method for focusing THz beams employs gold-plating parabolic mirrors, which are bulky and very expensive. In addition, these mirrors have fixed quasi-optical parameters such as focal lengths and beam waists. Compact and tunable focusing elements are highly desired in advanced THz imaging and spectroscopy systems (e.g., imaging for different depths of a sample).

In this poster, we propose to develop and demonstrate photo-induced Fresnel-zone-plates (FZPs) for tunable THz beam focusing. In our previous research, we have found that photo-induced free carriers in unpatterned high-resistivity silicon could be employed to spatially modulate THz beams. This same mechanism can be adopted to generate virtual and universally tunable FZPs using commercially available digital light processing (DLP) projector. This kind of FZPs are not only inexpensive and compact, but also offer enhanced tunability for beam focusing without requiring any pre-patterned circuits, masks, or mechanical movement (i.e. dynamic beam focusing). The basic focusing principle involved in FZPs will be studied and an experimental setup suitable for beam focusing demonstration will be presented. The potential challenges in implementing this approach and its future prospects will also be examined.
Conversion of a greenhouse gas, methane, into a versatile chemical, methanol, is currently an expensive two-step process. A more economical process of direct conversion of methane to methanol would be highly desirable and allow more efficient transportation and storage of a readily available energy supply. Unfortunately, current metal catalysts prefer activating the C-H bond in methanol rather than in methane. Methanol is quickly converted to unwanted products such as CO₂. To solve the problem, research is focused on modifying catalysts to lower the activation barrier to form methanol while raising the barrier to form CO₂.

Screening large amounts of metal catalysts in an experimental lab is expensive and time consuming. Computers save time and money by calculating energies more quickly and allowing researchers to identify trends. Models were created using GaussView software, and energies calculated using Density Functional Theory (DFT), and Basis Set LanL2DZ. Nine metals in various configurations were evaluated. Results show that the dissociation energy of the C-H bond in methanol is lower than the dissociation energy of the C-H bond in methane matching experimental results of metal catalysis.

Additionally, periodic trends are not consistent in metal clusters of very small size. Future research options include (1), increasing the metal cluster size until consistent results can be obtained, (2) investigating results on a variety of metal alloys, and (3) investigating results with a variety of pre-adsorbed atoms, such as oxygen.
Poster Presentation

Modification of Curcuminoids and Studies on their Modes of Action

Ryan Soheim
Erin Berube
Advisor: Masato Koreeda, Dept. of Chemistry, University of Michigan

Turmeric (Curcuma longa), a plant indigenous to South Asia, has widely been used in Indian and Middle Eastern cuisine, and has been a major part of alternative medicines throughout Indian history. Recently, the major constituent of turmeric, curcumin, has gained extensive research popularity for its use in the potential treatment of an array of different diseases (including cancer, diabetes, Alzheimer’s, and other chronic illnesses). This project proposes affecting the ability of various curcumin’s keto-enol tautomerization using its C4-modified derivatives.

Scheme 1. Keto-enol tautomerization of curcumin

Scheme 2. Overview of the reactions

1. Acetylation
2. C4-Modification
3. Hydrolysis

1. R₁ = Ac, R₂ = H
2. R₁ = Ac, R₂ = CH₃, F, CH₂CH₂
3. R₁ = H, R₂ = CH₃, F, CH₂CH₂
The year 1848 was one that overwhelmed Italy, as well as all of Europe. Revolutions overtook Europe. Italy became a sovereign country between 1860 and 1870 and there came to be very well known history that was written soon after. My work seeks to recapture the local and regional meanings of the revolutions of 1848 on the Italian Peninsula and there were many. For example, the January Revolution of 1848 in Palermo occurred because Sicilians did not want the royal courts to be brought back by Ferdinand IV. They revolted because, as Sicilians, they desired a more liberal constitution; Italian unification was not a priority at that moment. However, the history written after this event points in the opposite direction. Following the events in Sicily, revolts took place in diverse parts of the Peninsula. Under Italian national historiography these revolutions in Sicily lost their local purpose, instead they were seen as the spark to a larger Italian unification movement. The histories of these revolutions were Italianized and the fragments were used to make an Italian history. The study shows an in-depth look at two sources of information: what was written in the time of the revolutions and the historiography that took place leading up to and after unification. History served a purpose in the Italian unification. My project how essential history was to the making of Italy.
Isolation of Antimicrobial Compounds from Red Oak (Quercus rubra L.) Acorns

Robert Stanley
Clayton Thomas

Advisors: Jeanne Romero-Severson, Shaun Lee, Dept. of Biological Sciences, and Viktor Krchnak, Dept. of Chemistry and Biochemistry, University of Notre Dame

Every year over 75,000 people become infected with Methicillin-resistant Staphylococcus aureus (MRSA) in the US alone. These bacterial infections are resistant to most current antibiotics, and are developing resistance to others faster than new antibiotics are being produced. This loss of viable antibiotics has caused researchers to revisit traditional sources of antimicrobial compounds; plants, animals and fungi. This research project is focused on investigating new antimicrobial compounds from the acorns of the northern red oak (Quercus rubra L.). Extracts of powdered acorns in water, ethanol, and ethyl acetate have all demonstrated activity against a variety of bacteria including MRSA and Streptococcus sp. We have partially purified the ethanol extract through multiple High Pressure Liquid Chromatography (HPLC) separations. These fractions have been tested for antimicrobial activity, and the most active portions have been further purified. Analytical data was recorded through Liquid Chromatography Mass Spectroscopy (LCMS) and Nuclear Magnetic Resonance (NMR). Multiple fractions of the ethanol extract have shown strong inhibition of MRSA implying that there are multiple antimicrobial compounds. Future work will focus on isolating the active compounds and devising a method of synthesis.
Breast cancer is the most common cancer and the second leading cause of cancer-related deaths among women in the United States. Early detection by mammography is the current gold standard in breast cancer screening and is considered to be the best hope for controlling the disease given a demonstrated decrease in breast cancer mortality. However, accurate detection of breast cancer is limited by the specificity and sensitivity of mammography. Therefore, breast tissue phantoms that mimic the size, shape, compressibility, and X-ray attenuation properties of the tissue components of the human breast are desired to evaluate a novel X-ray contrast agent for targeting breast microcalcifications. Current phantoms used for training surgeons and radiologists consist of gelatin or high density polymer and mimic the low attenuation of the adipose tissue component of breast tissue. However, these models fail to take into account fibroglandular tissue, or tissue abnormalities such as microcalcifications, or tumor masses. The goal of this project was to fabricate and test appropriate materials to mimic both the adipose and fibroglandular components of the human breast while accommodating injections of mineral compositions used to model microcalcifications and targeted X-ray contrast agents. Candidate phantom materials were adopted from previous tissue-equivalent substitutes found in literature. Each material was fabricated in varying concentrations, imaged by micro-CT, and injected with hydroxyapatite mineral compositions. Phantoms were polymerized within a custom aluminum mold that was designed and fabricated to mimic human breast anatomy. The polymerization of acrylamide in N,N’-methylene-bis-acrylamide, water, ethylene glycol and other suspending materials exhibited X-ray attenuation similar to the fibroglandular components of the breast. Additionally, ethanol-based gels consisting of water, ethanol, and polyvinyl alcohol exhibited X-ray attenuation similar to adipose tissue. Thus, by combining the two materials an advanced breast phantom was prepared for investigating the detection of breast cancer. Future work will include optimization of X-ray attenuation of existing materials and searching for other acceptable material substitutes.
The damaged zebrafish retina regenerates retinal neurons from Müller glia cells in the inner nuclear layer of the retina, which dedifferentiate, reenter the cell cycle to make neuronal progenitor cells (NPCs) that continue to proliferate and differentiate into the missing neurons. It was recently demonstrated that Notch signaling acts in the undamaged zebrafish retina to keep the Müller glia from reentering the cell cycle. When Notch signaling is inhibited by injection of the γ-secretase inhibitor RO4929097, the Müller glia in the undamaged zebrafish differentiate and reenter the cell cycle (Conner et al. 2014). Thus, activation of the Notch receptor is required to keep the Müller glia from reentering the cell cycle in the undamaged retina. To identify which of the four different zebrafish Notch receptors functions in regulating retinal regeneration and the cells that they act in, I performed in situ hybridizations on light-damaged Tg(gfap:EGFP)nt11 transgenic retinas, which express EGFP in all the Müller glia. The notch1a and notch1b genes are expressed in a subset of the Müller glia after 36, 51, and 68 hours of constant light damage. At 96 hours of light treatment, notch1a and notch1b expression is observed in the outer nuclear layer of the retina, where the neuronal progenitors have migrated to regenerate the lost photoreceptors, while the Müller glia lack notch1a and notch1b expression. In summary, we do not detect any significant difference in the expression of notch1a and notch1b and their expression pattern is inconsistent with acting to maintain the Müller glia in a quiescent state in the undamaged retina.
Oral Presentation

*Coupling Algorithm for Sp(3,R) Irreducible Representations*

James St Germaine-Fuller  
Anna McCoy  
Advisor: Mark Caprio, Dept. of Physics, University of Notre Dame

The nuclear symplectic model based on Sp(3,R) — the smallest algebra that contains both the shell model Hamiltonian and the rotor algebra — connects the microscopic shell model to collective rotational behavior and naturally extends the Elliot SU(3) model to multiple shells. However, Sp(3,R) is only an approximate symmetry of the nucleus, where the symmetry can be broken by spin-orbit interactions, tensor force interactions, and pairing. The Hamiltonians in most physical situations will break the Sp(3,R) symmetry, causing their eigenstates to become linear combinations of symplectic irreducible representations (irreps). Calculations with those eigenstates will then involve multiple irreps. We report a computer algorithm for coupling symplectic irreps that should assist in performing such multi-irrep calculations and facilitate computing symplectic coupling coefficients.
Biomedical research and therapeutics have created a high demand for recombinant proteins. Many human proteins that have biomedical significance are glycoproteins, such as antibodies. Current systems used for recombinant protein synthesis cannot produce higher eukaryote glycoproteins with the correct carbohydrate side chains at greater than 30 to 40% of the total product composition. Differences in glycosylation can cause an immunogenic response making the proteins unfit for clinical use. Thus, it is important to find a system that cannot only create recombinant proteins in a time and cost effective manner, but can also correctly glycosylate those proteins. The silkworm, *Bombyx mori*, has been proposed and tested as a potential system because it can synthesize and secrete large amounts of protein in its silk glands making it ideal for the mass production of recombinant proteins. We hypothesize that human N-glycosylated proteins can be synthesized with greater homogeneity for the preferred product and easily recovered from silkworm cocoons.

A plasmid containing anti-EGFR (Cetuximab) was constructed and microinjected into silkworm eggs utilizing the piggyBac transposon for transformation. The plasmid was first injected into a control parental line and then crossed into the GG1 line which has been genetically engineered to include mammalian N-glycosylation enzymes N-acetylglucosaminyl-transferase II (Gn-TII) and galactosyltransferase (Gal-T). Fluorescent eye markers have indicated that the plasmid is expressed in the silkworms and preliminary analysis of protein expression in the cocoons provides evidence that the antibody is present. Further work will be done to confirm these results and provide more in depth analysis of the antibody expression.
A changing climate necessitates the ability to model the effects of future temperature shifts. The Eastern tiger swallowtail butterfly, *Papilio glaucus*, is a useful model organism for the study of these effects. In order to have an effective model, it is important to know its life cycle, including in what stage it is induced to diapause. We conducted an experiment to determine the stage in which this occurs. *P. glaucus* larvae were initially placed into a long day (16 hour photoperiod) treatment and different groups were moved to a short day (12 hour photoperiod) treatment at each successive instar, including the five larval instars as well as the pupal stage. We hypothesized that induction to diapause occurs in the larval stage. Individuals were observed either to direct develop into an adult butterfly or diapause. We found that all individuals that entered the short day treatment before 15 days, or the third instar, diapaused. We can therefore infer that the larvae are induced to diapause around 15 days of age, or in the third larval instar, in response to shortened photoperiod. This knowledge can be used to improve future model systems by specifying when the organism is sensitive to photoperiod, and also to compare the physiology of diapause among different species.
Nitric oxide (NO) is involved in several biological processes in humans, but the overproduction of NO has detrimental consequences for human health. On the contrary, denitrifying organisms effectively detoxify NO. Fungi detoxify NO by reduction to nitrous oxide by a Cytochrome P450-type nitric oxide reductase (Cyt. P450nor). The active site of this enzyme contains a ferric heme $b$ center coordinated to a proximal cysteinate ligand. In the proposed mechanism of this enzyme, the ferric heme binds NO and is subsequently reduced to an iron(II)-HNO complex. To investigate whether iron(II)-HNO complexes are catalytically competent intermediates in the mechanism of Cyt. P450nor it is insightful to use model complexes. Here, we synthesize cobalt(II) porphyrin complexes and react these complexes with nitrosoalkane compounds (RNO), where the nitrogen atom is substituted with an R group. First, tetraphenylporphyrin (TPP$^{2-}$) is synthesized by refluxing pyrrole and benzaldehyde in propionic acid. Then, the porphyrin is metallated with cobalt(II) sulfate heptahydrate in refluxing DMF to produce cobalt(II) tetraphenylporphyrin. Next, [Co(TPP)] is reacted with nitrosoalkane compounds, nitrosobenzene (PhNO) and 2-methyl-nitrosopropane (tBuNO) to synthesize [Co(TPP)(PhNO)$_x$] and [Co(TPP)(tBuNO)$_x$] (where $x = 0-2$). These reaction products were characterized using UV-vis, $^1$H-NMR, and IR spectroscopy.
Tuberculosis (TB) is an infectious disease caused by *Mycobacterium tuberculosis* (MTB), which is estimated to have claimed 1.3 million lives in 2012. Co-infection with HIV is a critical issue, and people with HIV are estimated to have accounted for 25% of the deaths from TB in 2012. Another even more important issue is the increasing prevalence (est. 450,000 cases in 2012) of multidrug-resistant strains of TB (MDR-TB and XDR-TB), which are much less effectively treated with current drug regimens. Rifampin is a key drug used to treat TB, and inhibits RNA transcription by targeting the RNA polymerase of MTB (MTB RNAP). The Garcia Lab has been investigating rifamycin-resistant (RifR) mutations in the β subunit of MTB and *Escherichia coli* (E. coli) RNAP and their interactions with structure-based, designed rifamycin analogs. While these RifR mutations do protect the organism from rifamycin inhibition, they exhibit “impaired fitness”. However, secondary mutations, which stabilize and compensate for this fitness defect under stringent growth conditions, have been discovered in the β’ subunit, encoded by the rpoC gene, of MTB RNAP. The purpose of this study is to investigate these secondary mutations in MTB and *E. coli* RNAP in vitro and how they compensate for the impaired fitness of the RifR RNAPs. Two compensatory mutations (β’V408G and β’F377L) have been introduced by site-directed mutagenesis into the rpoC gene of *E. coli* RNAP. The rpoC genes, containing the mutations, were then subcloned into the wild-type and three RifR RNAP expression plasmids. These mutant *E. coli* RNAPs are currently being expressed and purified, and their transcriptional activities and inhibition by the rifamycin analogs are being characterized. It is hypothesized that these compensatory mutations will increase activity of the RNAPs containing the RifR mutations. This study is directed towards the ultimate goal of developing an improved rifamycin analog that will be active against the RifR RNAP, and thus will lead to an effective treatment for MDR/XDR-TB.
Trimethoprim (TMP) is an antifolate drug used to treat malaria, but resistance to the drug has developed. To overcome this, a novel strategy has been developed to conjugate TMP to a dendrimer that uses van der Waals interactions to increase binding. A synthetic approach to obtain these conjugates is to make amine and azide functionalized TMP molecules by the conversion of the central methoxy group on the TMP to a primary amine. The amino-TMP can then be converted to azide-TMP. These functionalized TMP molecules are fully characterized by NMR and mass spectrometry. Then, they can be conjugated to either a carboxylic acid focal point of a dendron through an amide coupling reaction or to a cyclooctyne functionalized dendrimer via a strain promoted azide alkyne cycloaddition (SPAAC).
Poster Presentation

Structure Based Functional Comparison of 3-deoxy-D-manno-oct-2-ulosonic Acid Transferase

Sierra Vanderkelen
Andrew Pratt
Advisor: Ronald Woodard, Dept. of Medicinal Chemistry, University of Michigan

A key player in the survival of pathogenic Gram-negative bacteria is the lipopolysaccharide. The first step in the formation of the core region of lipopolysaccharide in all known gram-negative bacteria is the addition of at least one 3-deoxy-D-manno-oct-2-ulosonic acid (Kdo) monomer to lipid IVA by the Kdo transferase, WaaA. This essential step in the pathway represents an attractive target for pharmaceutical research. This research seeks to identify the differences in functionality of the diverse subclasses of WaaA. With this knowledge comes the possibility of the creation of novel vaccines and a deeper understanding of WaaA. An in vivo screening method to identify functionality by complementation for bifunctional WaaA proteins has been developed. We are using crystallography to determine structural differences between subclasses of WaaA proteins.
Poster Presentation

Ultrafast Time-resolved Spectroscopy of Donor-Acceptor Photovoltaic Copolymers Based on 2,6-di(thiophen-2-yl)benzo[1,2-b:4,5-b']difuran

Ricardo Javier Vazquez  
Oluwasegun Adegoke  
Advisor: Theodore Goodson III, Dept. of Chemistry, University of Michigan

The potential optoelectronic applications of organic polymers in polymer solar cells (PSC) have stimulated academic and industrial studies in the last decade. Organic polymers have advantages such as ease of chemical synthesis, ease of fabrication of large-area films using low-cost solution processing techniques and ease of manufacturability of lightweight and flexible organic polymer-based devices over their inorganic counterparts. Recent studies suggest that design of organic polymers based on alternating electron donor-acceptor moieties is a compelling and effective way to alter the optical and electronic properties of organic polymers. Donor-acceptor conjugate polymers show beneficial properties such as broad absorption band, appropriate offset of LUMO levels from fullerene acceptors, low-lying HOMO levels and high charge-carrier mobilities. Therefore, four new conjugated polymers featuring electron donor-acceptor moieties were investigated for their lifetime dynamics and two photon absorption capabilities. The polymers were based on 3,7-didodecyl-2,6-di(thiophen-2-yl)benzo[1,2-b:4,5-b']difuran (BDF) as the donor and 3,6-di(thiophen-2-yl)-1,4-diketopyrrolo[3,4-c]pyrrole (TDPP) or 3,6-di(2-furanyl)-1,4-diketopyrrolo[3,4-c]pyrrole (FDPP) as the acceptor. The diketopyrrolopyrrole co-monomers have two different alkyl chains to enhance solubility. The lifetimes of excited states of the polymers were measured through the time correlated single photon counting (TCSPC) and femtosecond up-conversion techniques which are capable of studying dynamics of excited state decay over timescales from femtosecond to nanosecond range. The polymers with 2-ethylhexyl side chain have relatively longer lifetimes than similar polymers with a tetradecyl side chain. The FDPP-containing polymers show higher molar extinction coefficients than the TDPP-containing polymers. The two-photon Excited Fluorescence (TPEF) method used for the measurement of two-photon absorption (TPA) cross-section, showed that the TPA cross-sections of FDPP-containing polymers were ten times higher than those of TDPP-containing polymers. This result indicates that FDPP-containing polymers have greater dipole moments and higher charge transfer character than TDPP-containing polymers. Therefore, FDPP-containing polymers have better potentials as solar cell materials.
Splitting water into oxygen and hydrogen using visible light has shown promise as an environmentally friendly and renewable process to store solar energy as hydrogen fuel. The reaction rate is limited by water oxidation, so many research efforts are focused on catalyzing this half reaction. The semiconducting material WO$_3$ has shown promise as a water oxidation photoelectrocatalyst due to its small band-gap of 2.7 eV and good stability at low pH. However, WO$_3$ photoanodes are not particularly selective for water oxidation; the Faradaic efficiency (product generated per equivalents of electrons reacted) for O$_2$ evolution is only 70%. The efficiency can be increased through loading a cocatalyst that is selective for O$_2$ evolution to the system. Iron oxyhydroxide (FeOOH), is a known electrocatalyst for water oxidation, and the specific aim of this work was to use FeOOH as a cocatalyst with WO$_3$ to improve selectivity. Here, FeOOH was photodeposited onto WO$_3$ electrodes through a pulsed current technique under illumination in the presence of 0.1 M FeCl$_2$, we are able to produce a film of FeOOH on the WO$_3$’s surface, which was characterized electrochemically and by SEM. Bulk electrolysis stability tests conducted in pH 4 KH$_2$PO$_4$ under 1-sun illumination indicate that these WO$_3$/FeOOH electrodes have Faradaic efficiencies as high as 98%, which is remarkable for WO$_3$ photoanodes. Current efforts are directed toward optimizing the FeOOH growth conditions to obtain complete film coverage of WO$_3$ in order to improve stability under neutral and basic conditions.
Finding optimal parameters for use of position-sensitive ionization chamber

Daniel Votaw
Mathematics and Physics
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This paper details work done in the development and testing of various components of what is to become an ionization chamber with two position-sensitive boards and a downstream scintillation counter. The ionization chamber is intended to be used for fast particle identification of high-current heavy ion beams. Work was supervised by Dr. Dan Bardayan and Dr. Patrick O’Malley of the Notre Dame Nuclear Science Laboratory (NSL). The design is loosely based on the design of another ionization chamber at Oak Ridge National Laboratory (ORNL). Optimal bias voltage and gas (P10) pressure for the electrodes were determined using a standard chamber and an α-source containing 148Gd and 228Th. A prototype for the 700 μm-diameter, gold-coated tungsten wire position-sensitive boards was built using a printed circuit board and 0.1 mm wire of the same kind.
Poster Presentation

Maximum Constraints of Resolution Detected in Planar (Xtreme) & Computed Tomographic (CT) X-ray Modalities

Justin Waller
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X-ray CT is a widely used technique that commonly utilizes anatomical imaging modalities for clinical, professional and research purposes. Computed Tomography is able to integrate three-dimensional data at high resolution with quick attainment to provide a non-intrusive human or specimen imaging platform. Imaging instruments and tools utilizing X-rays were probed for limits of resolution to assess their utility for anatomical imaging. Computerized designs interfaced with 3D-printing enabled the production of resolution phantoms for the acquisition of imaging resolution limitations. Acquisitions of images via In-Vivo Xtreme integrated with the components of the Albira PET/SPEC/CT Imaging system allowed for execution of manipulative actions to efficaciously reconstruct imaging settings to affirm numerical values of limitation. American wire gauge (AWG) copper wires of varying diameter were effectively utilized in the attenuation of X-rays to exploit and confirm resolution constraints. Full width half max (FWHM) values were derived from line intensity profiles, for highly accurate values of the limitations that are existent in imaging equipment and instruments.
Non-coding RNAs play crucial roles in a multitude of biological processes such as translation, messenger RNA (mRNA) splicing and regulation of gene expression. Riboswitches are regulatory elements found mainly in the 5’ untranslated regions of numerous bacterial mRNAs capable of modulating gene expression in response to the binding of cellular metabolites. Riboswitches comprise two functional components: a ligand binding aptamer domain and an expression platform whose conformation decides the fate of gene expression. Despite its smallest size among all reported aptamers, the Bacillus subtilis (Bsu) preQ1 (pre-queuosine) riboswitch boasts precise control of the expression of genes involved in the biosynthesis of queuosine, and high selectivity towards preQ1 over other non-cognate but similar ligands in vivo. Previous studies indicated that the Bsu riboswitch binds closely related ligands including preQ0 and guanine with similarly favorable affinities. However, the mechanism of how the aptamer differentiates between these ligands and their effect on the aptamer conformational dynamics remained elusive and can reveal to what extent near-cognate ligands stabilize the folded state to affect gene regulation. Here, we use smFRET to study the effects of preQ0 and guanine in comparison to preQ1 on the kinetics of the Bsu aptamer folding. Our preliminary data show that in the presence of Mg2+, under both saturating and non-saturating concentrations, preQ0 stabilizes the folded state more potently as compared to guanine. However, and rather surprisingly, in the absence of Mg2+, guanine tends to stabilize the folded state more efficiently than preQ0. The effect of Mg2+ on the folding pathway was also investigated. In the absence of Mg2+, the aptamer folds mainly via the induced fit mechanism whereas folding through conformational selection assumes dominance in the presence of Mg2+. Notably, our preliminary data indicate that at high ligand concentrations and in the presence of Mg2+, the aptamer folds via a major induced-fit mechanism. Our work clearly demonstrates the major roles played by Mg2+ in altering the effectiveness of a ligand in stabilizing the folded conformation and in deciding the folding pathway of the RNA.
The Arctic participates in unique photochemical processes during the polar springtime due to reactions on land based snow and sea-ice snowpack. Atmospheric ozone and mercury levels have been observed to reach near zero levels during a process involving photochemical reactions with bromine in the snowpack and atmosphere known as bromine activation. The surface snowpack has recently been identified as the primary source of reactive bromine to the Arctic troposphere when the snowpack is acidic and has a high bromide/chloride ratio. To examine the variability of the chemistry of snow across the Arctic, snow pack was collected from various sites and depths across the Arctic Ocean and nearby coastal areas during the spring of 2013 and 2014. The snow was melted prior to pH measurement and ion chromatography (IC) analysis for the quantification of sodium, ammonium, calcium, magnesium, chloride, bromide, nitrite, nitrate, sulfate and phosphate. The measured snow chemistry will be used to predict whether bromine activation will take place in the snowpack at the collection site during polar sunrise. Additionally, air mass trajectory modeling was used to determine the effect of water leads in the sea ice on nearby snow chemistry when plotted against MODIS satellite sea-ice images on the day of collection. Using this information, we can better predict whether the snowpack will produce bromine for ozone and mercury depletion.
70-kDa heat shock proteins, also known as Hsp70, assist in many protein homeostasis processes. One major process that it contributes to is the refolding of misfolded and aggregated proteins. Over expressed forms of Hsp70 can have an effect on the folding of certain proteins. Cancer cells need chaperones, such as Hsp70 and Hsp90, to facilitate uncontrolled cell growth and to buffer oncoproteins with destabilizing mutations. XIAP is an enzyme that can stop apoptic cell death and is found in cancer cells as overexpressed or in high proportion. Previously, it has been shown that chemical inhibition of Hsp70 proteins can cause degradation of XIAP in cancer cells. To study the change in XIAP levels in response to genetic inhibition of Hsp70, two different Hsp70 constructs, Hsp72 and Hsc70, were created using site-directed mutagenesis. These constructs were designed for mammalian overexpression and each contain an N-terminal FLAG tag. We then engineered E175S point mutants in each Hsp70 gene. This mutation creates a dominant-negative form of Hsp70 with increased affinity for substrate proteins. The mutant enzymes were then overexpressed into cancer cells. Once in the cancer cells, the levels of XIAP were examined through a Western Blot. Through Western Blot analysis we are able to observe that there is an increase in XIAP levels when the overexpressed Hsp70 constructs are added to cancer cells.
Poster Presentation

*Exploring Proteinase-activated Receptor-2 (PAR2) Mediated p65/p50 Canonical Pathway Activation in Oral Squamous Cell Carcinoma*

Russell Williams III  
Jeffrey Johnson  
Sharon Stack  
Adviser: Sharon Stack, Dept. of Chemistry and Biochemistry, University of Notre Dame

The family of transcription factors known as nuclear factor kappa-light-chain-enhancer of activated B cells (NFκB) has been linked to cellular transformation, proliferation, apoptosis suppression, invasion, angiogenesis, and metastasis which makes it a strong investigative target for studying mechanisms and pathways involved in tumorigenesis (Aggarwal, 2004; Basseres, Baldwin, 2006). Furthermore, PAR2 is a G-protein-coupled receptor activated by protease cleavage that is upregulated in oral cancer and has been shown to activate the NFκB pathway (Cunningham et al. 2005). Inflammation – in which PAR2 signaling plays a key role – has been shown to be linked to cancer initiation and progression. We are investigating the link between pro-inflammatory signaling by PAR2 and OSCC progression. Additionally we are interested in the role of kallikrien-5 (KLK5), a secreted enzyme also upregulated in oral cancer and reported to cleave and activate PAR2, in this pathway. This relationship is especially important in oral cancer due to the connection of NFκB to tumorigenesis and the upregulation of both PAR2 and KLK5 we have observed in oral cancer cell lines. Using different activators of PAR2 (KLK5, trypsin, and the activating peptides SLIGRL-NH2 and 2f-LIGRLO-NH2), along with inhibitors of downstream targets (pertussis toxin for G-protein signaling and sc-514 and SB 747651A for NF-κB signaling), we will investigate PAR2 signaling through the NF-κB pathway – with a particular interest in NFκB-κB target gene activation.
Fiducial markers can be used to describe anything that marks a fixed point of reference or measure in image processing. They have a number of purposes across various fields, from Quick Response (QR) code recognition to implantation for localized radiation therapy. The PADs Project is an interdisciplinary project at Saint Mary’s College and the University of Notre Dame that uses colorimetric chemical reactions on Paper Analytical Devices (PADs) to indicate the presence of ingredients commonly used in counterfeit pharmaceuticals. In the PADs Project, fiducial markers are used to indicate the location of chemical reactions on lanes. In computationally analyzing the PADs, a more unique, colored fiducial marker was needed to orient the image and identify lane location for analysis. Details of the design and implementation will be discussed.
Poster Presentation

*Photovoltaics: Cu$_2$S Synthesis, Solar Cell Efficiencies, and Applications*

Mark Wilson
Jeffrey Christians
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While there are currently many different methods of solar cell production, the need to make them as efficient as possible is the primary goal. In the same manner as energetic efficiency, economic and materialistic efficiency are factors that are playing ever-increasing roles in the manufacturing schema of the solar cell. Economically manufacturing solar cells requires integrating low cost, effective components, such as Cu$_2$S. Cu$_2$S’s low cost and relatively simplistic synthesis make it an interesting candidate as a “hole conductor”. Determining Cu$_2$S’s level of functionality and obtaining higher levels of solar cell efficiency serve as the primary objectives of this research. From this, the concepts of solar energy and the general working principles of a solar cell will be taught and demonstrated in the high school classroom.
Oral Presentation

High Purity Germanium Detectors and Angular Distribution of $^{27}$Al(p,γ)$^{28}$Si

Andre Wilson
Advisor: Edward Stech, Dept. of Physics, University of Notre Dame

The purpose of this research was to study germanium detector systems, and to calculate and compare absorption ratios of $^{27}$Al(p,γ)$^{28}$Si. Work with the Georgina detectors, including energy calibrations and work with software and hardware logic, provided the necessary background and experience with high purity germanium detectors and angular distribution of gamma rays. The knowledge taken from work with the Georgina detectors was then applied to the analysis of $^{27}$Al(p,γ)$^{28}$Si. Previous experimental data of $^{27}$Al(p,γ)$^{28}$Si was analyzed using the $E_p = 1778.9$ keV resonance. The data used was taken from a 2010 experiment that was completed in the Nuclear Science Laboratory at the University of Notre Dame using the 4MV KN particle accelerator. A 1977 paper by A. Anttila and J. Keinonen with analysis of the same reaction using the $E_p = 992$ keV resonance was used for energy calibration and gamma energies. Peak fitting and background reduction of the spectra were completed using analysis software, jtek. Angular distribution ratios from a $^{56}$Co source were used for the normalization of the $^{27}$Al data. Angular dependent absorption factors were used to analyze the angular distribution of γ-rays from the $^{27}$Al beam target. With these absorption factors, relative γ-ray intensity measurements of $^{27}$Al(p,γ)$^{28}$Si were calculated.
We are studying the intercellular behavior of the bacteria *Myxococcus xanthus* to detail the connection between the polarity of *M. xanthus* and local concentration of the protein RomR within the cell. RomR is known to localize in the poles of *M. xanthus* with one pole showing a higher concentration of RomR than the other. The difference in relative RomR concentration may infer the orientation of polarity in *M. xanthus*. In our study, information about the bacteria movement and RomR concentration throughout the cell was collected by using fluorescent microscopy for RomR-GFP images (green) and bright field microscopy for images of the whole cell (black and white). Image analysis is used to quantify the relative RomR concentration at the poles, and this information is compared to cell movement and directionality.
The development of alternative energy has been focused on the harvesting of energy, however, it is now clear that energy storage is another key component to our energy future. Various techniques of storing renewable energy have been proposed. One promising method is the utilization of high energy density capacitors.\textsuperscript{1,2} Traditionally, this field has been dominated by the use of inorganic ceramic materials, but there is a clear need to develop other materials that provide improved performance, especially for hybrid electric devices.\textsuperscript{1} One such material discovered by our group is the organic dielectric material: hyperbranched copper phthalocyanine (HBCuPc) dendrimer. This poster will highlight some of the properties that make this material desirable as well another material that includes doping an organic polymer with these classical ceramic materials.

Generation of TALEN-induced Aaop1 Knockout in *Ae. aegypti*

Jeff Yu
Michelle Whaley
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It is estimated that each year over 100 million people are affected by the mosquito-borne tropical diseases dengue fever and yellow fever. Studying the primary vector for these diseases, the mosquito *Ae. aegypti*, and more specifically its visual system may provide novel avenues for vector control and preventing disease transmission. TALEN site specific endonuclease technology has been used to achieve a knockout of Aaop1, the main rhodopsin in *Ae. aegypti*, as a means to impair the visual system. The goal is to create and breed an Aaop1 homozygous knockout line, verify the rhodopsin knockout and use these mosquitoes in behavioral assays to determine the role of vision in vector competence. A TALEN endonuclease targeting of the Aaop1 gene was used to promote recombination at the gene. A repair plasmid, which contains regions of homology to Aaop1, an attP recombination site and a one base-pair deletion results in a frameshift mutation upon recombining into the genome through homology-direct repair. To determine the efficacy of the TALEN reaction and the genetic status of the mosquitoes, numerous pair mates were established and diagnosed by PCR. This analysis showed that the insert successfully recombined and introduced the attP site into the genome. After assaying multiple generations of heterozygous pair mates, we determined that the attP was not targeted to Aaop1 through homology-directed repair. The data showed that an M13 DNA sequence site, adjacent to the Aaop1 insert and not expected to be present in the genome after homologous recombination, was still associated with the attP insert. Thus, the repair plasmid recombined at an ectopic site, not at the Aaop1 gene. Splinkerette PCR analysis is currently being used to determine the exact recombination site of the repair plasmid sequences. Our current efforts to establish knockout of the Aaop1 gene will use a CRISPR endonuclease in place of the TALEN endonuclease.
Poster Presentation

Molecular Characterization of Dissolved Organic Matter in Cloud Water from Whiteface Mountain (NY)

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Zhuoyu Peng
Eric Boone
Julia Laskin
Alexander Laskin
James Dukett
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Clouds play a major role in the Earth’s climate through participation in the hydrological cycle (precipitation) and chemical cycles, as well as by affecting the total albedo of the planet. The cloud formation process, in which supersaturated water condenses onto cloud condensation nuclei (CCN), makes cloud droplets an unique environment for chemical reactions. Very few studies have investigated high molecular weight organic compounds dissolved in cloud water, and these compounds are hypothesized to contribute a significant mass fraction of atmospheric aerosols upon cloud droplet evaporation. Multiple cloud water samples were collected at Whiteface Mountain in New York from September 10-11 2013 during near-continuous cloud cover to study the organic composition of cloud droplets. Electrospray ionization (ESI) coupled with LTQ-Orbitrap mass spectrometry was used to provide detailed molecular characterization due to its high resolution and mass accuracy. NOAA HYSPLIT backward air mass trajectory analysis was used to determine the source regions of the particles forming the sampled cloud droplets. Inorganic ion concentrations (e.g. sulfate concentration) were compared with corresponding organic composition (e.g. sulfate-containing organics) to examine potential trends. Meteorological parameters (e.g. cloud, liquid water content) were also studied for a better understanding of the cloud environment. Understanding the organic composition of cloud water will help determine the dominant chemical processes in clouds.
Oral Presentation

Effect of Antagonists on Heteromerization of NMDA Receptor Ligand Binding Domains

Ning Zhou
Francis Castellino
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N-methyl-D-aspartate receptor (NMDAR) is a glutamate- and voltage-gated cation channel expressed throughout the central nervous system. NMDAR exists prevalently as a hetero-tetramer composed of two glycine binding GluN1 subunits and two glutamate binding GluN2 subunits. NMDAR plays a crucial role in neuroplasticity, learning, and memory. Although structure based understanding of ligand binding to GluN1 and GluN2A has been reported, their inter-subunit associations and the role of ligands in modulating the functional behavior of these domains needs better understanding. Here we studied the interaction between the ligand binding domains (LBDs) of GluN1 and GluN2A subunits and how they are affected by two potent antagonists of NMDAR namely, DCKA and AP-5. We expressed the LBDs in Drosophila S2 cell expression system and purified them to homogeneity for our studies. Using analytical ultracentrifugation, we show that DCKA negatively affected the heteromer formation of GluN1 and GluN2A while AP-5 did not. Our findings provide new detail to the mechanism of action of the NMDAR antagonists with respect to hetero-oligomerization of the receptor domains. We are also studying the ligand induced domain interactions by heterologously expressing NMDAR channels in HEK cells with mutations at the interface of the LBDs and analyzing channel activity using patch clamp electrophysiology. Our studies on the inter-subunit associations and the role of antagonists in modulating the functional behavior of NMDAR will ultimately help towards devising methods to counter its dysregulation in several neuropathies like stroke and epilepsy.