
# The Dr. James Girard Summer Undergraduate Research Experience (SURE)

## 2023 Symposium

## Lewis University

## Wednesday, August 9, 2023

SURE

LEWIS UNIVERSITY
*A Catholic and Lasallian University*

# Schedule

## Location: AS-158-A

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|---|---|---|
| 8:30am–9:05am | **Breakfast and coffee served in University Dining Room** | |
| 9:05am–9:10am | **Welcome: Dr. Brittany Stephenson** | |
| 9:10am–9:20am | **Opening remarks: Dr. Christopher Sindt** | |
| 9:20am–10:20am | Session 1 | **Elisa Morales**: *Characterizing Biogenic MnOx Particles Produced by Pseudomonas putida MnB1 and Its Catalytic Activity Towards Water Oxidation*<br>**Kristen Ess**: *A Mathematical Model of Disease Spread Incorporating the Environment and Interactions in Healthcare Settings*<br>**Nina Demma**: *Using a Molecular Approach to Compare Bacterial Communities Found in Zebra Mussels and Daphnia Microbiomes*<br>**Daisy Collazo**: *Firearm Safety Education in Perinatal and Pediatric Settings* |
| 10:20am–10:30am | **Break** | |
| 10:30am–10:45am | **President remarks: Dr. David Livingston** | |
| 10:45am–11:30am | Session 2 | **Aiysha Shamsi**: *Evaluating Cyclin D3 as a Transcriptional Regulator During Neutrophil Differentiation*<br>**Jacob Prince**: *An Application of Optimal Control Theory to a Compartmental Model of COVID-19 Transmission*<br>**Tatiana Cahue**: *Stimuli-Responsive $CeO_2$ Removal via Surface Redox Modulation During Shallow Trench Isolation (STI) post-Chemical Mechanical Planarization (p-CMP)* |
| 11:30am–12:45pm | **SURE Luncheon in University Dining Room and Group Picture** | |
| 12:45pm–1:30pm | Session 3 | **Austin Rockaitis**: *Synthesizing and Modifying ASOs by Replacing Oxygen with Sulfur to Produce ASOs with Better Binding Efficiencies and Greater Stability*<br>**Caitlin Lamirez**: *Multidimensional Analysis of an RNA Dataset using High Performance Computers*<br>**Laila Mahrat**: *Impartial Geodetic Achievement and Avoidance Games Played on Connected Graphs* |
| 1:30pm–1:40pm | **Break** | |
| 1:40pm–2:25pm | Session 4 | **Anthony DiBenedetto**: *Application of Machine Learning for Optimization and Rapid Process Development in Atomic Layer and Chemical Vapor Depositions*<br>**Rebecca Rozhon**: *Copper Chelation via Quinolines as a Therapeutic Approach in a C. elegans Model of Alzheimer's Disease*<br>**David Abrutis**: *Verilog to Rust Translator* |
| 2:25pm-2:30pm | **Closing remarks: Dr. Brittany Stephenson** | |

# List of Abstracts

## Session 1

### Characterizing Biogenic MnOx Particles Produced by *Pseudomonas putida* MnB1 and Its Catalytic Activity Towards Water Oxidation

***Elisa Morales***

**Mentor**: Dr. Kari Stone

Mn-oxidizing microorganisms oxidize environmental Mn(II) producing Mn(IV)-oxides. *Pseudomonas putida* MnB1 is a widely studied organism for the oxidation of manganese (II) to manganese (IV) by a multicopper oxidase. The biogenic manganese oxides (BMOs) produced by MnB1 and similar organisms have unique properties compared to non-biological manganese oxides. Along with an amorphous, poorly crystalline structure, previous studies have indicated that BMOs have high surface areas and high reactivities. It is also known that abiotic Mn-oxides promote oxidation of organics and have been studied for their water oxidation catalytic function. MnB1 is grown and maintained, and subsequently transferred to culturing media containing manganese (II) salts to observe the oxidation of manganese (II) to manganese (IV). The structures of these manganese (IV) oxides have been characterized by scanning electron microscopy, energy dispersive X-ray spectroscopy, inductively coupled plasma optical emission spectroscopy, powder X-ray diffraction, Brunauer-Emmett-Teller surface area, and their properties assessed for catalytic functionality towards water oxidation. We have shown that we can achieve water oxidation by both whole cell catalysis and purified BMOs leading to further investigations of water oxidation compared to abiotic Mn(IV) oxides.

### A Mathematical Model of Disease Spread Incorporating the Environment and Interactions in Healthcare Settings

***Kristen Ess***

**Mentor**: Dr. Cara Sulyok

*Clostridioides difficile* (*C. difficile*) has been the leading cause of infectious diarrhea and one of the most commonly-obtained infections in United States hospitals. Those infected could have contracted *C. difficile* due to interactions with a surface or person harboring the spores spread by the disease. Patients that are infected with *C. difficile* spread these endospores which have proven to be difficult to remove from the hospital environment. The mathematical model developed uses a system of differential equations including different transmission routes such as healthcare workers, doctors, and low- and high-touch frequency fomites, objects likely to carry infection. The results from this model can be applied by those in the healthcare field into their practice in order to lessen the spread of *C. difficile* in healthcare settings.

## Using a Molecular Approach to Compare Bacterial Communities Found in Zebra Mussels and Daphnia Microbiomes

***Nina Demma***

**Mentor**: Dr. Jerry Kavouras

Zebra mussels, or *Dreissena polymorpha*, are bivalve mollusks that are an invasive species and have major effects on food web interactions. *Daphnia dentifera* are microcrustaceans that serve as indicator species and are important in food webs. Zebra mussels and Daphnia compete for algae. A microbiome is a community of microbes living on or within an organism. Bacteria in the microbiome can aid in digestion, provide resistance to infections, help to break down toxic chemicals, and help the host tolerate stressors by fostering their innate immune systems. The purpose was to compare bacteria living on daphnia, on the zebra mussel, and in the water using a molecular approach. The hypothesis is that the zebra mussels contributed bacteria to the microbiome of the Daphnia via the water column. The setup for the experiment consisted of control mesocosms with daphnia and experimental mesocosms with zebra mussels and daphnia, which were maintained over time. DNA extraction, PCR, RISA, and gel electrophoresis were used to analyze the microbial communities. The nucleotide sequence between the 16s-23s intergenic spacer region was amplified, because it varies in length and nucleotide sequence among species. Therefore, band patterns observed on agarose gels may be used for comparing microbial communities. Preliminary results indicate that the protocol is successful, however, there needs to be stronger amplification of the intergenic space to obtain a more visible band. Future work will look at re-amplifying the PCR product to increase product yield.

## Firearm Safety Education in Perinatal and Pediatric Settings

***Daisy Collazo***

**Mentor**: Dr. Hannah Klein

The Centers for Disease Control reports that nine children and teens die daily from firearms, often in homes with unsecured or improperly stored guns. Without education about proper firearm storage, increasing numbers of children are accidentally shot or killed by other kids or suffer self-inflicted injuries. With nearly 400 million firearms being owned across the country, there exist numerous chances for children to access these weapons. Preventing these deaths can be done by prioritizing gun safety education in perinatal classes and pediatric settings. In this study, Illinois parents participated in online surveys to collect their opinions on firearm education in these healthcare settings. Parents reported a lack of information on firearm storage safety and safety around children in healthcare settings, though a majority said they'd be comfortable with hearing about firearm safety in these settings. Healthcare workers took part in interviews to share their opinions and experiences regarding firearm safety education during appointments. Professionals expressed uncertainty about appropriate resources that could address the problem effectively. The findings highlighted the importance of promoting proper gun security measures and a need for more education. In conclusion, parents are receptive to gun safety education in pediatric and prenatal settings while healthcare workers lack proper education about the information that they can provide to improve patient and family education.

# Session 2

## Evaluating Cyclin D3 as a Transcriptional Regulator During Neutrophil Differentiation

***Aiysha Shamsi***

**Mentor**: Dr. Sarah Powers

Cyclin D3 is a protein essential for cell proliferation at the $G_1$ to S phase transition, where it binds to cyclin-dependent kinases, and promotes DNA synthesis. Cyclin D3 is implicated as a transcriptional regulator, controlling transcription through an indirect mechanism. To understand this function more thoroughly, quantitative PCR (qPCR) was used to measure the expression of certain genes as the level of cyclin D3 present varied using a neutrophil differentiation model. HL-60 cells are a human cell model capable of transitioning from an undifferentiated progenitor state (uHL-60) to a differentiated neutrophil state (dHL-60) when treated with DMSO. The total RNA was extracted from cells and converted into cDNA. Several genes hypothesized to be sensitive to cyclin D3-impacted gene transcription, including *AGL*, *HECTD1*, *APPBP2*, and *BRIP1*, were evaluated by qPCR and compared across the developmental states. These gene targets were also evaluated in HL-60 cells that were ectopically expressing cyclin D3. Through the UCSC Genome Browser, the promoter regions of 38 genes that are thought to be regulated by cyclin D3 were analyzed, and transcription factors that could work indirectly with cyclin D3 to regulate gene expression were identified. By collecting data from both qPCR and the UCSC Genome Browser, we were able to determine the effect cyclin D3 had on gene expression for our target genes and identify potential transcription factor partners participating in this process.

## An Application of Optimal Control Theory to a Compartmental Model of COVID-19 Transmission

***Jacob Prince***

**Mentor**: Dr. Brittany Stephenson

The COVID-19 pandemic has had a massive socioeconomic impact on countries all over the world and is one of the most severe global health crises of the past 100 years. In order to describe, better understand, and predict the spread of the virus, mathematical models have played an important role. In this work, we consider a compartmental model that uses a system of ordinary differential equations to model COVID-19 transmission based on data from the Chicagoland area. To this model we apply optimal control theory in order to determine the time-varying optimal vaccination rate that minimizes both disease prevalence as well as the "costs" associated with vaccination. In this case, "cost" is a broad term considering time, money, and effort to vaccinate. We then solve the optimality system, which consists of the compartmental model, an adjoint system, and characterization of the optimal control, using a Forward-Backward Sweep method, an iterative method that solves the system using a fourth-order Runge–Kutta scheme. The system can then be updated with different parameters and weighting coefficients to determine the optimal time-varying vaccination rate under different conditions, such as times of outbreak or increased susceptibility.

## Stimuli-Responsive $CeO_2$ Removal via Surface Redox Modulation During Shallow Trench Isolation (STI) post-Chemical Mechanical Planarization (p-CMP)

***Tatiana Cahue***

**Mentor**: Dr. Jason Keleher

As transistor miniaturization continues to extend Moore's Law into the future of technology, the demand for high-efficiency device manufacturing processes has increased drastically in recent years. More specifically, a critical step in preparing integrated circuits (ICs) and logic devices is Chemical Mechanical Planarization (CMP), which relies on a delicate balance of chemical and mechanical parameters to achieve angstrom-level surface uniformity and ultimately allows for increased transistor packing density. A sub-area of CMP that has gained significant attention is Shallow Trench Isolation (STI), which involves the isolation of electrically active components by removing the bulk oxide (i.e., tetraethyl orthosilicate (TEOS)) overburden from the deposition process. During polishing, chemical slurries comprised of $CeO_2$ nanoparticles, rate enhancers, selectivity and rheology modifiers, and pH adjusters are utilized to activate the oxide layer and consequently remove material. The STI removal mechanism, known as the chemical tooth model, involves the nucleophilic attack of $CeO_2$ nanoparticles at surface defect states (i.e., oxygen vacancies ($O_{vacs}$)) and resultant dative Ce-O-Si bond formation, which makes the surface redox state of $CeO_2$ (i.e., $Ce^{3+}/Ce^{4+}$) a key driver for oxide-nanoparticle interactions. It is well known that $Ce^{3+}$ nanoparticles contain a higher concentration of $O_{vacs}$, which enhances the material removal rate (MRR). However, the hard adsorption properties of $CeO_2$ have resulted in the demand for a more efficient post-CMP (p-CMP) cleaning process for TEOS that promotes increased $CeO_2$ removal without inducing secondary defects (i.e., scratching, dishing, corrosion, etc.). Current industry-standard methods involve using a polyvinyl alcohol (PVA) brush to transport harsh chemistries to contaminated surfaces under high shear force (SF). Additionally, the use of megasonic energy is an emerging non-contact cleaning mode that relies on generating reactive oxygen species (ROS) (i.e., cavitations) to induce particle removal. Previous work has shown that supramolecular additives improve overall particle removal efficiency (PRE) when implemented in traditional PVA brush cleaning due to their ability to encapsulate and charge-flip $CeO_2$ nanoparticles while reducing SF. As a result, this research investigates a combinatorial approach to PVA brush cleaning utilizing megasonic energy to release Fenton catalysts from polymer capsules, which aid in the production of ROS through $H_2O_2$ decomposition. Initial results have shown that, by increasing the concentration of ROS during cleaning, a $Ce^{3+} \rightarrow Ce^{4+}$ transition occurs on the surface of adsorbed $CeO_2$, enhancing overall PRE.

# Session 3

## Synthesizing and Modifying ASOs by Replacing Oxygen with Sulfur to Produce ASOs with Better Binding Efficiencies and Greater Stability

***Austin Rockaitis***

**Mentor**: Dr. Daniel Kissel

Machado Joseph Disease is an autosomal dominant genetic disease caused by excessive glutamine repeat in the Ataxin protein. The Ataxin protein aggregates and causes neurodegeneration leading to paralysis. To produce mutant protein, Antisense oligonucleotides (ASO) were synthesized to bind to the mRNA produced from the mutant gene and alter processing to generate a truncated protein. The oligonucleotides will then be introduced into cultured human cells to cause skipping of an exon and halt the production of the protein containing the excessive repeat. The conventional synthesis method is a five-step approach, this synthesis adds an additional step, sulfurization. Sulfurization uses a reagent called DDTT, which replaced the reactive oxygen with reactive sulfur. Making this modification, however, leads to a greater electronegativity resulting in better binding to RNA by the ASO. Some oligonucleotides need functional groups added to further enhance their stability. In this project pure ASOs of high yield were created, with the correct sequence and a variety of sulfur modifications to determine which ASO best treats Machado Joseph disease.

## Multidimensional Analysis of an RNA Dataset using High Performance Computers

***Caitlin Lamirez***

**Mentor**: Dr. Michael Lewis

For geneticists and immunologists, understanding correlations between particular genes in gene networks is vital in order to understand the functionality of our genetic codes. However, with over 25,000 protein-encoding genes within the human genome, it would be a computationally exhaustive task to process, as it requires significant time and computational power. To address this, we propose utilizing high-performance computing systems, specifically supercomputers, to analyze partitions of the dataset amongst multiple processors. Once partitioned, we can use data mining algorithms, such as k-means clustering or Apriori, and show the resulting images. These resulting images would ultimately make up a “visualization book”, in which the end user is able to visualize the dimensions of the dataset for easy content analysis. However, one challenge from the genomic dataset stems from the 200 columns representing tissue lineages. Typically, algorithms that are multidimensional are computationally expensive, therefore, we had to come up with an algorithm that works on 200 dimensions. Dimensionality reduction methods, such as Principal Component Analysis (PCA), would not be an option due to the risk of data loss. Therefore, we created the “Subdimensional Consensus” algorithm, which involves taking a consensus from all the 2-dimensional cluster combinations within a column to determine the outlying RNA values, which can suggest gene expression. Overall, by harnessing the power of distributing computing and creating the “Subdimensional Consensus” algorithm, we aim to enhance geneticists’ and immunologists’ ability to discover vital genetic associations."

### Impartial Geodetic Achievement and Avoidance Games Played on Connected Graphs

***Laila Mahrat***

**Mentor**: Dr. Marie Meyer

Buckley and Harary introduced two types of impartial geodetic games played on connected graphs called the achievement and the avoidance games. In this research, we introduce and solve a new variation of these games on various graph families. First, an impartial game is a 2-player game in which the possible moves are the same for each player in any position and no position can be visited twice. We play our combinatorial games on graphs; a geodesic on a graph is the shortest path between two vertices, and the geodetic closure of a set is the set of vertices contained on geodesics between all pairs of vertices in the set.

Both games proceed as players alternate choosing vertices on the graph, and in the original games, the geodetic closure is computed after each turn. In our new games, we look at the vertex-set geodesic, which is the union of the set and the shortest path between the vertex and the set. That set updates after each turn, and we call that set $Q$. The player that selects a vertex such that $Q = V$ wins our achievement game, where $V$ is the set of all vertices on a graph, and the player that chooses the last vertex such that $Q \neq V$ wins our avoidance game. We solved these new games on the following graphs: paths, complete graphs, complete bipartite, cycles, and wheels.

## Session 4

### Application of Machine Learning for Optimization and Rapid Process Development in Atomic Layer and Chemical Vapor Depositions

***Anthony DiBenedetto***

**Mentor**: Dr. Sam Abuomar

Atomic layer deposition (ALD) is a thin film fabrication technique that relies on self-limited surface reactions, pivotal in semiconductor miniaturization and other high-precision applications. Despite its utility, the quality of ALD processes significantly impacts the properties of the resulting thin films, and this necessitates costly and time-consuming experimental work to evaluate new ALD processes. This quality is quantified by predicting the standard deviations of film thickness, with lower deviations signifying better process quality. To accelerate this process, we leverage machine learning to rapidly assess the quality of ALD processes. Using a synthetic dataset generated to simulate various non-ideal ALD processes, we compared and evaluated the performance of different models. These models, include Random Forest Classifier (RFC), Support Vector Machines (SVMs), and K-Nearest Neighbor (KNN). Each sample is labeled as an ideal self-limited or a non-ideal ALD process. To confirm our findings from these models we added Gaussian noise to the data and performed a similar analysis. Additionally, we developed an artificial neural network (ANN) and a convolutional neural network (CNN) to predict the standard deviations of film thickness resulting from each ALD trial. Our CNN and ANN models achieved great results on the test data, so they can be used as a reliable tool to predict the standard deviation values.

## Copper Chelation via Quinolines as a Therapeutic Approach in a *C. elegans* model of Alzheimer's Disease

***Rebecca Rozhon***

**Mentor**: Dr. Mallory Havens

The leading hypothesis for Alzheimer's Disease (AD) has traditionally focused on aggregating Amyloid-$\beta$ into amyloid plaques. However, all therapeutics targeting amyloid plaques have been unsuccessful in clinical trials or had limited efficacy. Therefore there is a need to explore alternative approaches to treating the disease. Many AD patients have dysregulation of metal ions, such as copper and zinc, in addition to accumulation of Amyloid-$\beta$. The interaction between Amyloid-$\beta$ and copper can result in the production of reactive oxygen species (ROS). ROS can cause damage to neurons and surrounding tissues resulting in degradation of the brain. Therefore, our work focuses on disrupting the interaction between Amyloid-$\beta$ and copper via chelation therapy to prevent ROS formation and, in turn, reduce neurotoxicity. In this study, copper chelation with a quinoline, specifically 2-Phenylquinoline (2TPIQ), aided in reducing the amount of ROS produced in the brains of *C. elegans*. Amyloid-$\beta$ aggregation, behavior, and lifespans of *C. elegans* were also observed. Our results suggest that copper chelation can potentially serve as an AD therapeutic.

## Verilog to Rust Translator

***David Abrutis***

**Mentor**: Dr. Lucien Ngalamou

Verilog is a hardware descriptive language that can be used to model digital systems. The System-on-Chip (SoC) industry has relied on hardware descriptive languages such as Verilog for hardware synthesis and verification. However, the implementation of simulated logic can't keep up with the complex growth of circuits and the industry's time-to-market pressure. Rust is a general-purpose language that offers a solution emphasizing performance and safety. The translation of Verilog into another language that can more efficiently and effectively verify hardware designs, can relieve time-to-market pressure, and keep up with the complex growth of SoC designs. This research project focuses on creating a Python program that can translate Verilog designs to comparable Rust programs for hardware verification purposes. The result can help build a foundation that will continue the development of a capable and efficient hardware verification tool that can use both the best formal and simulation verification methods to ensure valid chip designs.

# List of Participants

## Students

| | |
|---|---|
| David Abrutis | Computer Science |
| Tatiana Cahue | Chemistry |
| Daisy Collazo | Criminal Justice |
| Nina Demma | Environmental Science |
| Anthony DiBenedetto | Computer Science and Data Science |
| Kristen Ess | Physics |
| Caitlin Lamirez | Computer Science |
| Laila Mahrat | Mathematics and Data Science |
| Elisa Morales | Biochemistry |
| Jacob Prince | Mathematics and Computer Science |
| Austin Rockaitis | Biochemistry |
| Rebecca Rozhon | Biology |
| Aiysha Shamsi | Biology |

## Faculty Mentors

| | |
|---|---|
| Sam Abuomar | Professor of Data Science |
| Mallory Havens | Associate Professor of Biology |
| Jerry Kavouras | Professor of Biology |
| Jason Keleher | Professor of Chemistry |
| Daniel Kissel | Associate Professor of Chemistry |
| Hannah Klein | Assistant Professor of Justice, Law, and Public Safety |
| Michael Lewis | Assistant Professor of Computer Science |
| Marie Meyer | Assistant Professor of Mathematics |
| Lucien Ngalamou | Professor of Computer Engineering |
| Sarah Powers | Professor of Biology |
| Brittany Stephenson | Assistant Professor of Mathematics |
| Kari Stone | Associate Professor of Chemistry |
| Cara Sulyok | Assistant Professor of Mathematics |

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- Dr. Scholl Foundation

## Lewis University Internal Supporters

- President, Dr. David Livingston
- Provost, Dr. Christopher Sindt
- Associate Provost of Research and Educational Effectiveness, Dr. Bill Chura
- Office of the Provost