April 6th – April 7th 2024

2024 AICHE MID-ATLANTIC REGIONAL CONFERENCE

Hosted by:

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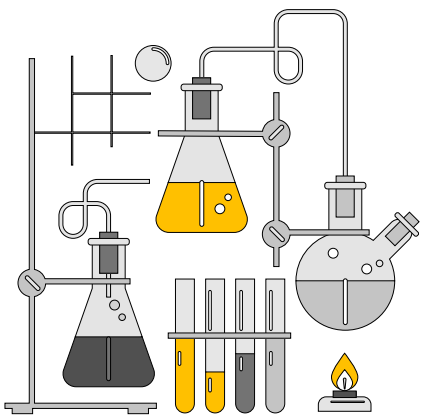

UMBC COLLEGE OF ENGINEERING & INFORMATION TECHNOLOGY

UMBC CHEMICAL BIOCHEMICAL AND ENVIRONMENTAL ENGINEERING

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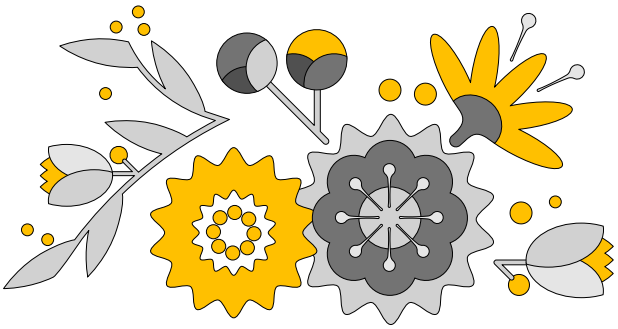
Welcome



AIChE Chapter at UMBC would like to welcome you to the **2024 Mid-Atlantic Regional Conference!**

We hope you will have a great experience with the competitions, workshops, and networking events our chapter has organized!

All inquires please reach out to:
aiche-conference2024@umbc.edu

Schedule

Saturday

Time	Event	Location
9:00 AM - 11:00 AM	Check-in	UC 3rd Floor Lobby
11:00 AM - 12:45 PM	Lunch & Keynote: **Mr. Pran Patel** Vice President of AstraZeneca's Global Engineering and Real Estate Division	UC Ballroom
1:00 PM - 1:50 PM	Workshop #1: **W.R. Grace** *Manufacturing Leadership Program*	ITE 104
2:00 PM - 2:50 PM	Workshop #2: **AstraZeneca** *Engineering for Patient Impact*	ITE 104
4:00 PM - 4:50 PM	Workshop #3: **CWIT, SWE, and W+GM at Virginia Tech** *Empowering Diversity: Advancing Women and Gender Minorities in STEM*	ITE 104
3:00 PM - 5:30 PM	Chem-E-Car Safety Inspection & Poster Presentation	UC 312
1:00 PM - 3:45 PM	Chem-E-Jeopardy Preliminary Rounds	ITE 2nd & 4th Floors
4:30 PM - 5:20 PM	Chem-E-Jeopardy Semi-Finals	ITE 2nd & 4th Floors
1:00 PM - 5:00 PM	Research Oral Presentation Competition	ITE 102
5:30 PM - 7:20 PM	Dinner & Keynote: **Dr. Sheares Ashby** President of the University of Maryland, Baltimore County	UC Ballroom
7:30 PM - 8:30 PM	Chem-E-Jeopardy Finals	ITE 104
9:00 PM - 10:30 PM	Student Networking and Social Event	Commons Skylight Room & Fireside Lounge

Schedule

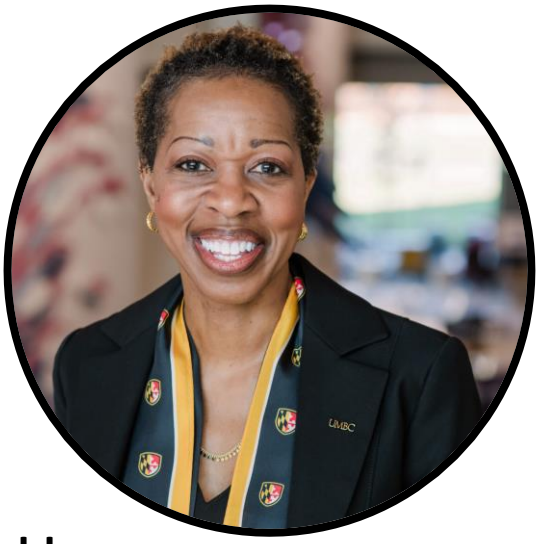
Sunday

Time	Event	Location
7:00 AM - 8:00 AM	Check-in	UC 3rd Floor Lobby
7:00 AM - 8:50 AM	Breakfast & Keynote: **Dr. Scott Banta** Professor & Chair of Chemical Engineering at Columbia University	UC Ballroom
9:00 AM - 9:50 AM	Presidents Meeting	UC 114
9:00 AM - 12:00 PM	Career Fair	RAC Arena Track
9:00 AM - 10:15 AM	Research Poster Competition (Session 1)	RAC Arena Track
10:30 AM - 11:45 AM	Research Poster Competition (Session 2)	RAC Arena Track
9:00 AM - 12:30 PM	Chem-E-Car Prep	RAC Arena Court
12:30 PM - 3:00 PM	Chem-E-Car Run	RAC Arena Court
12:00 PM - 1:00 PM	Pizza Lunch	UC Ballroom/RAC
10:30 AM - 11:20 AM	Workshop #4: **UMBC** *Ace the Graduate Application Process*	ITE 104
1:00 PM - 3:00 PM	Workshop #5 **AIChE** *Career Discovery*	UC 114
3:30 PM - 4:30 PM	Closing Award Ceremony	UC Ballroom

ITE: Information Technology & Engineering
UC: University Center
RAC: Retriever Activities Center

Keynote Speakers

Mr. Pran Patel
AstraZeneca
Vice President of Global Engineering and Real Estate Division



Dr. Valerie Sheares Ashby
University of Maryland, Baltimore County
University President

Dr. Scott Banta
Columbia University
Chair of Department of Chemical Engineering

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Chem-E-Jeopardy

Time: 1:00 PM – 5:20 PM (Saturday)
Location: ITE

ITE 227

Prelim 1	Prelim 2	Prelim 3
Bucknell 1	JHU 1	JHU 1
NJIT	CCNY 1	VT 2
SBU	PSU 2	Bucknell 1

ITE 229

Prelim 1	Prelim 2	Prelim 3
Bucknell 2	NJIT	RU
JHU 1	Rowan	CCNY 2
PSU 1	UMBC 1	PSU 1

ITE 231

Prelim 1	Prelim 2	Prelim 3
YSU	UMBC 2	SBU
Rowan	Bucknell 2	JHU 2
VT 1	CCNY 1	CCNY 1

ITE 233

Prelim 1	Prelim 2	Prelim 3
JHU 2	Bucknell 1	YSU
VCU	SBU	VCU
UMBC 1	YSU	UMBC 1

ITE 237

Prelim 1	Prelim 2	Prelim 3
UMBC 2	VT 2	PSU 2
PSU 2	PSU 1	NYU
CCNY 1	JHU 2	Bucknell 2

ITE 456

Prelim 1	Prelim 2	Prelim 3
VT 2	NYU	VT 1
CCNY 2	VT 1	NJIT
NYU	VCU	UMBC 2

Semi-Finals

ITE 227	ITE 229	ITE 231
Seed 1	Seed 2	Seed 3
Seed 4	Seed 5	Seed 6
Seed 9	Seed 8	Seed 7

Seeds are decided by prelim scores, and ties will be decided by total amount of cash accumulated.

ITE: Information Technology & Engineering

Chem-E-Car Teams

Time: 9:00 AM – 3:00 PM (Sunday)

Location: RAC Arena Court

John Hopkins University – *Hy-Speed Steed*

University of Maryland, Baltimore County – *VoltMaxing*

University of Maryland - College Park – *Dona-tudo*

University of Delaware – *Blue Lightning*

University of Pittsburgh – *Molar Express*

University of Pittsburgh Johnstown – *Hydro-Mobile*

Lehigh University – *The Packer Express*

Bucknell University – *H2Go*

Pennsylvania State University #1 – *Flint*

Pennsylvania State University #2 – *Car 2*

Carnegie Mellon University – *Twilights Gleam the Squeakuel*

Rutgers University – *Carbie*

New Jersey Institute of Technology – *Hylander*

Youngstown State University – *Pushin' Pete*

West Virginia University – *Mountaineer Car*

Virginia Tech – *Bruce Force*

Stony Brook University – *Catbus*

The City College of New York – *VitaVroom*

New York University – *Voltimus Prime Formic*

RAC: Retriever Activities Center

Oral Presentations

Time: 1:00 PM – 5:00 PM (Saturday)
Location: ITE 102

Melisa Bilgili – New Jersey Institute of Technology
Computational Analysis of N_8 Stabilized Isolated Single Atom Catalysts for Electrochemical Reduction of CO_2

Evalynn Ellison – University of Maryland, Baltimore County
A Synthetic Data Generator to Accelerate Machine Learning Algorithm Development

Yuseong Oh – Johns Hopkins University
Engineering Pan-Reactive VEGF Antagonists to Treat Neovascular Eye Diseases

Abdulla Alqallaf – Virginia Commonwealth University
Staying thermodynamically Consistent on VLE Prediction via Machine Learning

Maryom Rahman – New Jersey Institute of Technology
A Novel Selector Valve for a Point-of-Use Peptide Synthesizer

Riordan Correll-Brown – University of Maryland, College Park
Low-pressure planarization of gallium arsenide growth substrates via halide vapor phase epitaxy

Rwaka Bruce Furaha – Virginia Tech
Thermo-mechanical Property for 3D printed Carbon-Fiber Reinforced Polyamide Composite

Nick DeVita – Bucknell University
Diffusion in Macroscopically Layered Polymer Gels

John Pazik – Rowan University
Machine Learning for Predicting Cradle-to-Gate Life Cycle Inventory (LCI) Data that enables Early-stage Sustainability Assessment

Steven Roth – Rowan University
Residence Time Distribution studies to compare Multi-scale Petroleum Pipeline Operations

ITE: Information Technology & Engineering

Poster Competition

Time: 9:00 AM – 11:45 AM (Sunday)
Location: RAC Arena Track

Session 1: 9:00 AM – 10:15 AM

1. Melisa Bilgili
2. Sean Curtis
3. Michal Luchowski
4. Ding Wang
5. Saung Oo May
6. Blerina Sehitaj
7. Ethan Bolinger
8. Chiad Onyeje
9. Richard Zhang
10. Terra Miley
11. Princeton Bijou
12. Natalya Brown
13. Jared R. Ericksen
14. Jarett Ren
15. Aubrey Carey
16. John Velkey
17. Shane M. Coudriet
18. Owen Gereds
19. Hayden Medlin
20. Barry Najarro-Blancas
21. Joseph Fink
22. Milo Barkow
23. An Dang
24. Raey Hunde

Session 2: 10:30 AM - 11:45 AM

1. Kennedy Tomlinson
2. Abhiraman Senthilkumar
3. Abigail Martin
4. William Chen
5. Connor Richeson
6. Ryan C. Zmarzlak
7. Yasmi Chibber
8. Elijah Kaplowitz
9. Briman Yang
10. Riley Szumachowski
11. Rwaka Bruce Furaha
12. Sara Avraham
13. Sachin V. Kammula
14. Fariha Agbere
15. Alexander Davis
16. Maya A. Fetzer
17. Summer Hensley
18. Nathaniel Glover
19. Emma Padros
20. Kasey Piper
21. Elias Gilotte
22. Meredith Morse
23. Joshua Zhou

RAC: Retriever Activities Center

Abstracts – Oral Presentation

Computational Analysis of N_8 Stabilized Isolated Single Atom Catalysts for Electrochemical Reduction of CO_2

Melisa Bilgili [1], Joshua Young *[,1]
[1] Department of Chemical and Materials Engineering, New Jersey Institute of Technology, Newark, NJ

In this work, two-dimensional N_8 polynitrogen with various single metal atom catalysts (SMACs) was investigated for the electrochemical reduction of carbon dioxide (CO_2RR), utilizing density functional theory (DFT) calculations. SMACs demonstrate a bright future in degrading CO_2 into valuable non-greenhouse gasses, addressing the demanding global issues of renewable energy and environmental damages caused by CO_2 emissions in the atmosphere. These catalysts are attractive because of their low cost, unique structure and properties, and high performance. The reduction of CO_2 to carbon monoxide (CO), formic acid (HCOOH), methanol (CH_3OH), and methane (CH_4) on N_8 functionalized with SMACs Pd, Ni, and Co was investigated. The effects of pH, solvent, and applied voltage were studied, aiming to reduce the reaction's high overpotential while achieving high reactivity and selectivity. On Pd-N_8, CO, HCOOH, and CH_3OH can be efficiently produced, with the reaction performing better under acidic conditions. The substitution of Pd by Ni and Co is found to alter reaction thermodynamics. This work provides an understanding and prediction of novel catalysts for the CO_2RR, which may be used to inform experimentalists for catalyst design and synthesis to help overcome the urgent challenges of climate change.

A Synthetic Data Generator to Accelerate Machine Learning Algorithm Development

Evalynn Ellison [1], Gene Austin Lee [2,3*], and Brandon DeKosky [2,3*]
[1] Department of Chemical, Biochemical and Environmental Engineering, University of Maryland, Baltimore County (UMBC)
[2] Department of Chemical Engineering, Massachusetts Institute of Technology (MIT), Cambridge, MA
[3] The Ragon Institute of Massachusetts General Hospital (MGH), MIT, and Harvard Cambridge, MA

Machine learning algorithms for antibody mutations are lacking in diverse datasets to learn from. Without high-quality datasets, the predictions made by these algorithms are inaccurate. The DeKosky Lab at MIT has established a high-quality dataset approach for anti-malaria antibody screening. However, these datasets are time-consuming to develop, as many experiments are required to gather a robust number of data points. The focus of the current project is to create a synthetic data generator to use to explore algorithm development and test parameters while waiting for the experimental data from antibody engineering efforts. The synthetic data generator uses Python to create mutations in the wild-type amino acid sequence across two different malaria antibodies. Mutated sequences are then randomly assigned a corresponding binding affinity. The program outputs a specified number of mutated sequences, each with a binding affinity. This synthetic data can then be used to explore different data representations and as trial data for machine learning algorithms. These algorithms can then be used to help create a machine-learning model for highly effective monoclonal antibody treatments.

Engineering Pan-Reactive VEGF Antagonists to Treat Neovascular Eye Diseases

Yuseong "Nick" Oh [1], Paul Sargunas [1], and Jamie Spangler [*,1,2]
[1] Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD
[2] Department of Biomedical Engineering, Johns Hopkins University, Baltimore, MD

Ocular neovascularization drives the pathogenesis of neovascular age-related macular degeneration (NVAMD) and diabetic retinopathy (DR), two leading causes of blindness in adults. Vascular endothelial growth factor (VEGF) ligands are major stimulants of neovascularization, and blocking the binding of VEGF to their cognate receptors (VEGFRs) has shown clinical benefits. Most FDA-approved VEGF-targeted therapies for use in treating NVAMD and DR block VEGF-A ligand activity (prominent regulators of blood vessel formation) by competitively inhibiting their signaling through VEGFRs on the surface of epithelial cells. However, VEGF-C is increasingly implicated in pathological neovascularization, and is found to be upregulated following anti-VEGF-A treatment, leading to therapeutic resistance. Moreover, VEGF-C is just as potent as VEGF-A in driving retinal neovascularization under hypoxic conditions. No current therapies bind both VEGF-A&C, which would provide a more complete blockade. We designed an error-prone mutagenic DNA library templated on domains 2&3 of VEGFR-2, which binds both VEGF-A&C. We then used yeast surface display directed evolution to isolate and characterize high-affinity clones that bind both VEGF-A&C, and further designed novel dual decoy receptor antagonists by fusing the binding domains of VEGFR-2&1 to a human antibody Fc domain. These promising proteins could act as superior therapeutics to treat neovascular eye diseases.

Abstracts – Oral Presentation

Staying thermodynamically Consistent on VLE Prediction via Machine Learning

Abdullah Alqallaf [1], and Charles McGill [*,1]
[1] Department of Chemical and Life Science Engineering, Virginia Commonwealth University,

Predicting Vapor-liquid-equilibrium (VLE) has been one of the most problematic and time-consuming issues in the chemical engineering field due to the wide variety of mixture properties and phenomena that govern those mixtures, which necessitates a proper way to predict such data to use for relevant processes such as process optimization in the industry. In this work, we utilize Chemprop, a software package that implements a D-MPNN (Directed Message-Passing Neural Networks) architecture to enable better molecular representation for the inputted chemicals denoted by Simplified Molecular-Input Line-Entry System (SMILES), which are converted to molecular graphs, and subsequently to molecular vectors after the message-passing phase. Three VLE predictive models were developed to demonstrate how machine learning performs regarding predicting VLE data of binary mixtures. Training data of more than 50,000 data points were used from a variety of datasets of diverse quality, which made it necessary to do quality assessment procedures before feeding the data points into the developed models to ensure that the integrity and reliability of the models are precise. By assessing the quality of the fed data, the risk of data contamination is minimized, which enhances the reliability of the predicted targets of the machine-learning model.

A Novel Selector Valve for a Point-of-Use Peptide Synthesizer

Maryom Rahman [1], Alexandra Griffith [2], Vivek Kumar [1,2], Nellone Reid [*,1]
[1] Department of Chemical and Materials Engineering, New Jersey Institute of Technology, Newark, NJ
[2] Department of Biomedical Engineering, New Jersey Institute of Technology, Newark, NJ

Recent innovations show that peptide therapeutics can treat various ailments like triple-negative breast cancer. Fundamentally, a peptide synthesizer sequences amino acids into a peptide through successive protecting and deprotecting of functional groups; however, it produces large amounts of hazardous waste (consisting of dimethylformamide, diethyl ether, etc.) and costs around $30,000 to operate. Hence, a point-of-use, miniature model can be innovated to produce peptides with less cost and waste. The miniature peptide synthesizer consists of 4 main parts: the outer shell, two selector valves, the reactor, and an electrical chamber. Innovations in the first selector valve are made to mitigate leakage issues from previous designs. In this iteration, a new state-of-the-art selector valve is fabricated utilizing Fusion 360 computer-aided design (CAD) software and stereolithography (SLA) 3D printing. This design applies a ball piston and a spring to open and close access to the outlet chamber, leading to a compact, cost-effective, and torque-dependent device. A prototype with eight inlets to one outlet will be tested for leaks over various solvents. A 32-inlet to-one-outlet model is currently being designed. With this innovation, peptides can be synthesized in areas without proximity to labs or hospitals, and cultivate more peptide therapeutic distribution.

Low-pressure planarization of gallium arsenide growth substrates via halide vapor phase epitaxy

Riordan Correll-Brown [1], John Simon [2], Aaron Ptak [2], Kevin Schulte [2], Jacob Boyer 2, and Anna Braun [2],
[1] Department of Chemical & Biomolecular Engineering, University of Maryland, College Park, MD
[2] National Renewable Energy Laboratory, Golden, CO, 80401

III-V solar cells demonstrate high efficiencies, high specific powers, and flexible structures. However, these solar cells are currently too expensive for widespread use, and are restricted to specialized high-energy demand applications. One of the key cost drivers for III-V photovoltaics are the gallium arsenide (GaAs) substrates upon which they are grown. Re-using these substrates for multiple rounds of growth could significantly lower the cost of III-V technology. Controlled spalling shows promise as a low-cost, high-throughput substrate reuse technique. However, controlled spalling of (100)-oriented GaAs substrates produces triangular facets on the substrate surface, presenting an obstacle to device growth. It is possible to planarize these substrates via halide vapor phase epitaxial growth (HVPE). Here, planarization behavior was investigated under low-pressure growth conditions. Pressure, temperature, AsH3 carrier flow, and GaCl flow were varied, and their respective effects on planarization behavior and growth rate were measured. Under low pressures, growth rate was found to be sensitive to GaCl flow and AsH3 carrier flow, while growth rate anisotropy was sensitive to GaCl flow and temperature. Overall, planarization metrics were lower than those achieved in an atmospheric-pressure HVPE reactor. Compared to atmospheric pressure, higher growth rates were achieved at low pressures, suggesting improved reactant utilization.

Abstracts – Oral Presentation

Thermo-mechanical Property for 3D printed Carbon-Fiber Reinforced Polyamide Composite

Rwaka Bruce Furaha [*1,2], Martin Etemadi [1,2], Justin Anderson [1,2] and Michael Bortner[1,2]
[1] Department of Chemical Engineering, Virginia Tech, Blacksburg, VA
[2] Macromolecules Innovation Institute, Virginia Tech, Blacksburg, VA

Carbon fiber reinforced composites are known for their stiffness and high specific strength. Current advancement in additive manufacturing enables 3d printed CFRPs with a controlled variation of fiber content and fiber directionality. However, the mechanical properties of 3D printed CFRPs exhibit high variability when compared to conventional CFRP fabrication approaches. As part of an effort to build a predictive model for thermo-mechanical properties of 3D printed CFRPs, this poster discusses the results obtained in the study of 3D printed carbon fiber reinforced nylon (CFRPs) parts with varying fiber content and fiber directionality. Samples were printed on a Markforged printer using 3 raster angles of 0,45-, and 90-degree angle. The fiber content was varied by changing the number of carbon fiber layers in samples. The printed samples were then evaluated using Dynamic Mechanical Analysis (DMA) and Differential Scanning Calorimetry (DSC). The results suggest that thermo-mechanical analysis can be used to predict and optimize the design of 3d printed CFRPs.

Diffusion in Macroscopically Layered Polymer Gels

Nick DeVita [1] and Kenneth P. Mineart [*,1]
[1] Department of Chemical Engineering, Bucknell University, Lewisburg, PA

Transdermal drug delivery is a vital mechanism for skin care, hormone replacement, and other biomedical applications. Organic polymer gels have been recently identified as candidates for this drug delivery mechanism. Our present work focuses on controlling model drug release rate in a layered polymer gel system consisting of multiple organogels and a polystyrene backing. Typically, one organogel contains a diffusion probe [AOT (sodium bis(2-ethylhexyl) sulfosuccinate)], tri-block copolymer, and an organic solvent whereas the other contains only tri- block copolymer and organic solvent. The tri-block copolymer forms a physically crosslinked network within the gels that consists of spherical polystyrene domains and a plasticized rubbery matrix consisting of ethylene-co-butylene and aliphatic mineral oil (organic solvent). The matrix phase is fluid-like and amenable to mass transport, which allows for probe diffusion. Using Fourier Transform Infrared (FTIR) spectroscopy, the overall probe release rate, which stems from this diffusion, can be tracked. We are interested in the comparison between the layered systems and a 'traditional' system with a single organogel containing the AOT diffusion probe. We also seek to investigate how changing the tri-block copolymer concentration of the barrier organogel layer - that which contains no AOT - changes the overall diffusion probe release rate.

Machine Learning for Predicting Cradle-to-Gate Life Cycle Inventory (LCI) Data that enables Early-stage Sustainability Assessment

John Pazik [1], Jared Longo [2], Matt Conway [1], Milo Barkow [1], Austin L. Lehr [1], Emmanuel A. Aboagye [1], Robert Hesketh [1] and Kirti M. Yenkie [*,1]
[1] Department of Chemical Engineering, Rowan University, Glassboro, NJ
[2] Department of Mechanical Engineering, Rowan University, Glassboro, NJ

Improving the sustainability of chemical processes is crucial for mitigating the effects of climate change. This can be accomplished through incorporating considerations for environmental impacts during the early stages of process design while modifications can still be easily made. To facilitate this, a machine learning algorithm was developed to predict cradle-to-gate life cycle inventory (LCI) data for both pre-existing and novel chemicals. The LCI data predicted by the algorithm focused on four endpoint and 12 midpoint environmental metrics, which served as model outputs. The algorithm employed an Artificial Neural Network method. It was fed 500 data points split between a training, testing, and validation set that consisted of a feature set containing molecular descriptors and thermodynamic properties, which served as model inputs. Following hyperparameter tuning, the algorithm's performance was assessed on the test set using the root mean squared error. In addition to the algorithm itself, a case study representing the extraction of polyphenols from wine pomace using acetone solvent was also implemented to demonstrate the utility of the LCI prediction algorithm in enabling the creation of a detailed cradle-to-grave Life Cycle Analysis. The values produced by the model agreed with the case study results reported in literature (Vega 2021).

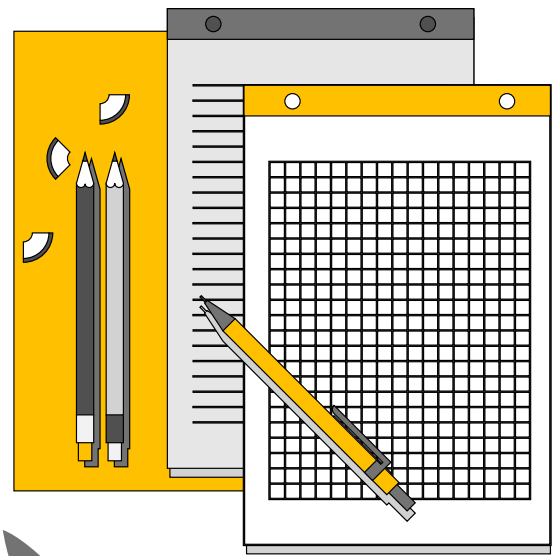
Abstracts – Oral Presentation

Residence Time Distribution studies to compare Multi-scale Petroleum Pipeline Operations

Steven Roth[1], David A. Theuma[1], Michael Fracchiolla[1], Emma Padros[1], Barnabas Gao[1], Robert P. Hesketh[1*], C. Stewart Slater[1*], Mariano Savelski, Kirti M. Yenkie[1*]

[1] Department of Chemical Engineering, Rowan University, Glassboro, NJ

In the oil industry, where multiple manufacturing processes often share the same pipelines and equipment, effective pipe flushing operations are critical to ensure product integrity. The pipeline flushing process occurs during a product change-over operation, where a new product flushes the remainder of the residual product through the line. This process generates a commingled oil which has limited use and low economic value. To understand the flushing operation, our team constructed a pilot plant that was a scaled-down version of a drum packaging line at a typical industrial facility. Multiple experiments were ran with both saltwater solutions and with oil, to create residence time distribution (RTD) models for the pilot plant. Conductivity and viscosity were the characteristics measured for saltwater and oil runs, respectively. The RTD curves generated from the model successfully mimic the curves generated from industrial scale data. These results will aid in the categorization of different types of oil, as well as the optimization of the flushing operation via different techniques, including the use of compressed air for residual product removal. Overall, results from this work will assist in developing strategies that can minimize the commingled oil formation, thus mitigating product losses during pipe flushing operations.



Abstracts - Poster Presentation

Computational Analysis of N_8 Stabilized Isolated Single Atom Catalysts for Electrochemical Reduction of CO_2

Melisa Bilgili[1], Joshua Young*[,1]
[1] Department of Chemical and Materials Engineering, New Jersey Institute of Technology

In this work, two-dimensional N_8 polynitrogen with various single metal atom catalysts (SMACs) was investigated for the electrochemical reduction of carbon dioxide (CO_2RR), utilizing density functional theory (DFT) calculations. SMACs demonstrate a bright future in degrading CO_2 into valuable non-greenhouse gasses, addressing the demanding global issues of renewable energy and environmental damages caused by CO_2 emissions in the atmosphere. These catalysts are attractive because of their low cost, unique structure and properties, and high performance. The reduction of CO_2 to carbon monoxide (CO), formic acid (HCOOH), methanol (CH_3OH), and methane (CH_4) on N_8 functionalized with SMACs Pd, Ni, and Co was investigated. The effects of pH, solvent, and applied voltage were studied, aiming to reduce the reaction's high overpotential while achieving high reactivity and selectivity. On Pd-N_8, CO, HCOOH, and CH_3OH can be efficiently produced, with the reaction performing better under acidic conditions. The substitution of Pd by Ni and Co is found to alter reaction thermodynamics. This work provides an understanding and prediction of novel catalysts for the CO_2RR, which may be used to inform experimentalists for catalyst design and synthesis to help overcome the urgent challenges of climate change.

Design and Assessment of Educational Crystallization Labs

Sean Curtis[1,2], Zachary Kazelskis[1] and Gerard Capellades*[,1]
[1] Department of Chemical Engineering, Rowan University

Despite being one of the most widely used and complex separation processes, crystallization has rarely been taught in chemical engineering education due to the lack of up-to-date textbooks and faculty expertise. The role of a Chemical Engineer has evolved significantly in the past few decades, but the separations curriculum has fallen behind. This project developed two different educational tools following the KEEN entrepreneurial mindset guidelines (Curiosity, Connections, Creating Value) to improve crystallization education in undergraduate programs. The first educational tool involved the optimization of a crystal growth children's science kit. Students went beyond the given instructions and created novel crystallization pathways to maximize yield. The methods and results were then presented to a faculty panel. The second tool is a traditional batch crystallization of acetaminophen in water. Students were encouraged to explore various methods of crystallization (cooling, antisolvent addition, seeding). The students were then assessed on their technical knowledge and their ability to form connections between different courses. The student evaluations were used to make future recommendations for lab implementation in other undergraduate programs. The results will be published as an Engineering Unleashed educational card for other faculty to use.

Elucidation of Ce/Zr ratio effects on the physical properties and catalytic performance of $Ce_xZr_{1-x}O_2$ catalysts

Michal Luchowski[1], Mohammed Sifat[1], Wenhui Jiang[1], Yunfan Lu[1], Gihan Kwon[2], Amol Pophali[1], Taejin Kim [1]
[1] Materials Science and Chemical Engineering Department, Stony Brook University
[2] National Synchrotron Light Source II, Brookhaven National Laboratory

Although cerium oxide (CeO_2) is widely used as a catalyst support, its thermal stability and limited defect sites should be improved. This study investigates the effect of Ce:Zr ratio on the physical properties of a series of $Ce_xZr_{1-x}O_2$(x=1, 0.9, 0.6, 0.5, and 0) support catalysts and the effect of a standardized surface density of copper on the support. The spectroscopic (e.g., Raman, XRD) and microscopic (e.g., SEM) characterization techniques were applied to evaluate the defect sites, crystallite size, lattice parameters, thermal stability, and chemical composition of catalysts. CO oxidation was used as a model reaction to describe the relationship between the structure and catalytic performance of each catalyst. Based on the characterization results, $Ce_xZr_{1-x}O_y$ could be a potential support for transition metals to catalyze various other industrial reactions. The inclusion of Zr into the structure of CeO_2 shrinks the overall lattice parameter of the catalyst, displays comparable catalytic ability compared to a pure ceria catalyst as well as enhancing the number of defect sites. Including surface species such as copper improves the catalytic activity of all the supports. The availability of commercially available $Ce_xZr_{1-x}O_y$ catalyst as support makes them a feasible choice for varying industrial processes.

Abstracts - Poster Presentation

Optimizing Pluronic F127-Alginate Multicomponent Hydrogel for Efficient Biomedical Applications in Wound Healing

Ding Wang[1], Tracy Colena[1], Hengwei Zhu, and Surita R. Bhatia*[,1]
[1] Department of Chemistry, Stony Brook University

Our research focuses on combining two types of hydrogels: alginate and Pluronic F127. Pluronic F127 is a special kind of hydrogel that reacts to temperature changes. When it's cold (below 10 ℃), it's a liquid that can adapt to the shape of a wound. But when it warms up (above 20-30 ℃), it turns into a gel, forming a protective barrier over the wound while staying safe for the body and keeping the wound moist. However, this gel can be easily distorted by forces. To make it stronger, we add alginate, which forms a supportive network for the F127. This mix creates pressure inside the hydrogel. But because it's sensitive, it takes more than two months to prepare the mixture. Our project aims to find a quicker way by adjusting the concentration of F127. We're testing how well the F127-Alginate mix responds to forces using a special machine called a rheometer. We'll compare different sets of data to see if we can cut down preparation time by at least a third without sacrificing the hydrogel's usefulness for medical purposes.

InFlux: a highly multiplexed neutralization assay to measure anti-influenza humoral immunity

Saung Oo May[1], Chun Huai Luo[2], Alexis S. Diaz[1], Christine Park[1], Andrew Pekosz[3], Heba H. Mostafa*[,2] ,H. Benjamin Larman*[,2]
[1] Department of Chemical and Biomolecular Engineering, Johns Hopkins University
[2] Department of Pathology, Johns Hopkins School of Medicine
[3] Department of Molecular Microbiology and Immunology, Johns Hopkins Bloomberg School of Public Health

Influenza A (IAV) presents a persistent public health threat despite annual vaccination efforts, with vaccine efficacy typically ranging from 20% to 60%. The challenge lies in the rapid mutation rate of the hemagglutinin (HA) protein, leading to escape mutations that compromise vaccine effectiveness. To address this, understanding population-level immunity is crucial. While current serological assays like ELISA provide valuable data on antibody abundance, they lack the ability to assess neutralizing activities, essential for estimating protective capacity.
To tackle this gap, we're developing a multiplexed neutralization assay capable of testing HA-neutralizing activities in human sera across 69 representative IAV strains. We're using a panel of single-replication cycle-restricted viruses, each carrying a distinct HA and identifiable by specific RNA barcodes. These barcodes reliably measure viral infectivity and determine neutralization titers. This innovative assay will allow rapid generation of population-level profiles of HA-neutralizing antibodies. These profiles will be crucial for evaluating the protective capacity against each HA at the population level, informing the development of more effective vaccines and therapeutics against IAV.

Electrochemical Self Discharge as a Crucial Phenomenon that Causes Capacity Fade in Aluminum-Quinone Battery

Blerina Sehitaj[1,] Harrison Asare[2,3,] George John [2,3,] Robert J. Messinger*[,4]
[1] Department of Chemical Engineering, Hostos Community College
[2] The PhD Program in Chemistry, The Graduate Center of the City University of New York
[3] Department of Chemistry & Biochemistry, The City College of New York
[4] Department of Chemical Engineering, The City College of New York

The rising demand for electric-powered devices requires designing energy storage technologies that promote a sustainable environment. Our strategy towards building sustainable energy storage technologies integrates the high capacity and abundant aluminum metal, and sustainable and tunable organic molecules as electrode materials for environmentally benign and energy-dense batteries. We synthesized a novel organic molecule, oxygen-bridged tetrakislawsone (OBTKL) from lawsone (an extract from henna plant) and subjected it to electrochemical screening in the aluminum battery systems. Cyclic voltammograms and galvanostatic cycling of the Al-OBTKL cells demonstrated pronounced reversibility at a higher voltage of 1.5 V vs Al/Al(III) compared to other quinones like anthraquinone (1.1 V vs Al/Al(III)). Our results demonstrated that capacity fading in Al-OBTKL cells arose from electrochemical self-discharge and not the dissolution of the organic material in the electrolyte. This work contributes important insights into capacity fading, a critical issue that challenges the field of organic batteries by providing practical design strategies to ameliorate cycling stability.

Abstracts - Poster Presentation

Storage buffer composition alters bacterial extracellular vesicle retention over time

Ethan Bolinger[1], Hayden Medlin[1], Robert D. Kirian[2], and Hannah Zierden[*,1,3]
[1] Chemical Engineering Department, University of Maryland, College Park, MD
[2] A. James Clark Department of Bioengineering, University of Maryland, College Park, MD
[3] Department of Obstetrics, Gynecology, and Reproductive Sciences, University of Maryland School of Medicine

Bacterial extracellular vesicles (bEVs) are lipid-bound nanoparticles produced by bacteria, enabling cross-kingdom communication between bacteria and mammalian cells. Recently, bEVs have been at the forefront of investigation as a novel drug delivery system due to their ability to facilitate cell to cell communication and bypass natural barriers within the body. Before these extracellular vesicles can be implemented as a drug carrier, we must first overcome production, storage, and scale-up challenges associated with biotherapeutics. In particular, post-isolation storage of the extracellular vesicles must be optimized for widespread clinical translation, where ultra-low freezer temperatures may not be feasible. Traditionally, bEVs have been stored in PBS at -80˚C, but this yields a relatively low recovery rate over long periods of time. Here, we investigate novel storage buffers to improve the retention and stability of bEVs over time. These results will garner and stimulate further research revolving around the post-isolation storage and subsequent drug delivery methods using bEVs, and transforming nanotechnology for human health applications.

How Many Passes Does it Take? An Investigation to Determine the Optimal Number of Liposome Extrusion Cycles

Kasey Piper[1], Kenneth Mineart[1]
[1] Chemical Engineering Department, Bucknell University

Liposomes are lipid-based nanoparticles commonly known for their drug carrying capacity and value in membrane and nanoreactor research. One commonly used method of fabricating liposomes of particular size is membrane extrusion where liposomes are pushed through a porous membrane and form smaller liposomes. However, the details pertaining to liposome extrusion, such as the number of passes, membrane pore sizes, and pre-extrusion sample preparation, vary between labs. The goal of this project is to establish a relationship between the number of passes through a track-etched, polycarbonate membrane, and the average diameter and lamellarity of extruded liposomes. To investigate, we extrude samples to different amounts varying from 1 to 1,000 passes and measure the average hydrodynamic diameter and diameter distribution of each using dynamic light scattering (DLS). We measure lamellarity with small angle x-ray scattering (SAXS) and cryogenic transmission electron microscopy (CryoTEM). When liposome size distribution and lamellarity data start to flatten out, it is suggested that extrusion has been completed, and further extruding would not change the liposome size and lamellarity. These results provide researchers with the optimal number of passes for liposome extrusion that will allow them to form ideal distributions in the shortest amount of time.

: Installing A Single Monomer Within Acrylic Polymers Using Photoredox Catalysis

: Richard Zhang[1], Jared G. Baker[1], and C. Adrian Figg[*,1]
[1] Department of Chemistry, Virginia Tech, Blacksburg, VA

The incorporation of a single functional group within a polymer chain is challenging. However, precisely installing a functional group within a polymer will provide a chemical handle to access defined architectures, morphologies, and mechanical properties. Most copolymerization approaches introduce a statistical distribution of monomers without control over the relative position of exactly one monomer. Single-unit monomer insertion (SUMI) reactions are a promising route to introduce functional groups within polymers because the poor reactivity of the monomer inhibits homopolymerization. This contribution details the development of SUMI reactions to place functional groups within polymer chains using reversible addition-fragmentation chain transfer (RAFT) polymerization. Herein, photo-induced electron/energy transfer (PET) enables the incorporation of one vinyl ether into polyacrylates synthesized via RAFT polymerization. Near-quantitative addition (>96%) of a single vinyl ether is achieved while retaining >99% of the thiocarbonylthio chain end. These results show that a single vinyl ether can be placed within acrylic polymers using PET catalysis. Precise placement of a single chemical handle within a polymer enables access to entirely new types of polymer architectures, and will allow for targeted functionalization of this chemical handle.

Abstracts - Poster Presentation

Genetically Encoded Fluorescent Magnesium Sensor To Be Used In An Industrial Cell-Free Bioreactor

Terra Miley[*,1,2], Govind Rao[*,1,2], Chad Sundberg[*,1,2], Elias Gilotte[1,2]
[1] Center for Advanced Sensor Technology
[2] Department of Chemical, Biochemical, and Environmental Engineering, University of Maryland Baltimore County

Cell free protein synthesis, otherwise known as in-vitro protein synthesis, provides opportunities for easy reaction condition manipulation, high-throughput potential, and rapid large-scale production, compared to live-cell bioreactors. With the application of a cell-free system, transcription and amino acid synthesis can be completed in the same compartment in cell-free protein synthesis, which makes the job of regulating magnesium, a cofactor, much more difficult, thus why a magnesium sensor would be essential to this process. Magnesium has various importance in cellular processes such as transcription, translation, energy metabolism, and replication. Cell-free protein synthesis is important in this process to be able to replicate and focus on the energy on production of a protein of interest. To address this challenge we have designed a fluorescent magnesium sensor to be used in a low cost fluidic chip. The sensor makes automated measurements from a bioreactor while immobilizing a fluorescent protein in microfluidic columns on Ni-NTA resin.

Evaluating Nutrient Levels in Select Lakes of the Romanian Danube Delta to Assess Ecological Health

Princeton Bijou[*,1], Hebatalla Kamaluddin-Nurdin[2], Niels Delbauve[3], Nikita Aksakow[4]
[1] Department of Chemical Engineering, Pennsylvania State University
[2] Faculty of Biology, University of Bucharest
[3] Faculty of Science, Université Libre de Bruxelles
[4] Brussels Bioengineering School, Université Libre de Bruxelles

The Danube Delta is the second-largest European river delta, mostly located in Romania. It is a World Heritage site, a UNESCO biosphere reserve, and a natural filtration system for water reaching the Black Sea. Though considered the best-preserved delta in the European continent, nitrogen and phosphorus levels have dramatically increased since the 1960s. These so-called “nutrients” are essential to ecosystem stability, but excesses can result in eutrophication. This study assessed the ecological health of select lake complexes in the Danube Delta by evaluating the spatial distribution of nitrogen and phosphorous species against standardized concentration matrices specified by the EU Water Framework Directive and the Danube River Basin Management Plan. Nutrient levels of water and sediment samples were measured for organic and inorganic species via spectrophotometry and a carbon/nitrogen analyzer. With results assessed with the context of local stressors, the study concluded that sites adjacent to higher anthropogenic and natural pressures exhibit diminished water quality and ecological health. To sustain the ecological health of the lakes within the Danube River Basin while meeting specific United Nation Sustainability Goals, it is suggested that viable sustainable agricultural and tourism practices be promoted and monitored by the Romanian government and related stakeholders.

Computer-verified BET analysis using the Lean Theorem Prover

John A. Velkey[1], Parivash Feyzishendi[1], Maxwell P. Bobbin[1], Tomás Skřivan[2], and Tyler R. Josephson*[,1]
[1] Department of Chemical, Biochemical, and Environmental Engineering, UMBC, Baltimore, MD
[2] Hoskinson Center for Formal Mathematics, Carnegie Mellon University

Because of the variety of computational tools/methods available for performing intensive calculations in engineering disciplines, inconsistencies between methodologies are common. For example, when adsorption data were sent to sixty-one different labs, there was wide variation in reported BET surface area, despite being a well-known calculation [1]. Consider the utility of computational programs that use functions with provable mathematics, that are “bug free” due to mathematical verification. To illustrate this, we use Lean 4 to write a computer-checked derivation of BET theory [2], and to write functions that regress BET parameters for given data. Lean 4 is a programming language with functionality as a theorem prover. Lean computing functions that use floating-point numbers cannot have proofs written on them, floats have inherent imprecision that makes writing proofs about their properties difficult. Reals can be subjects of proofs, but because they have infinite decimals, they cannot be utilized by computing programs. To achieve verified scientific computing in Lean, we introduce a method using polymorphism to connect proofs about real-valued functions to computations using the same functions with float-typed inputs. We use the functions to analyze datasets from [1], perform BET regression, and compare our results to those previously reported.

Abstracts - Poster Presentation

Dielectric and Mechanical Characteristics of Polyamide-Silicon Dioxide Nanocomposites

Jared R. Ericksen[1] ,Sean F. Lawton[1], Nicholas R. Mahon[2], Max P. Coraggio[3], John P Terifay[3], Michael Smith[1], Diana Martines-Castro[1], Paul M. Maienza[3], Wei Xue[3]
[1] Department of Chemical Engineering, Rowan University
[2] Department of Electrical and Computer Engineering, Rowan University
[3] Department of Mechanical Engineering, Rowan University

Nanocomposites have emerged as a promising area of research in recent decades due to their ability to improve the properties of host materials. Nanocomposites for cryogenic applications have gained significant attention for their potential in high-temperature superconducting (HTS) power transmission systems. However, exposure to low temperatures has detrimental effects on the mechanical properties of the material, limiting their applications. This necessitates the use of thermally stable high-quality dielectrics, which can be quantified through electrical and tensile testing. This paper discusses the preparation of poly(pyromellitic dianhydride-co-4,4'-oxydianiline), amic acid solution, and SiO2 nanoparticles through a sol-gel process to create PA/SiO2 thin films. The team has performed a multitude of AC and DC dielectric tests and tensile tests at room temperature. The results of this research can help improve the understanding of these composites and their potential for use in cryogenic applications.

Closed-Loop Materials Discovery for Multi-Principal Element Alloys

Jarett Ren[1], Maitreyee Sharma Priyadarshini[1], Eddie Gienger[2], and Paulette Clancy[*,1]
[1] Department of Chemical and Biomolecular Engineering, Johns Hopkins University
[2] Johns Hopkins University Applied Physics Laboratory

Advanced functional materials have widespread applications in energy, health, and space exploration, but their discovery is limited by a large combinatorial space that is expensive to characterize experimentally or computationally. In particular, high-hardness multi-principal element alloys (MPEAs) are desirable for their high strength-to-weight ratios, but synthesizing and testing them is costly. To address this problem, we developed PAL 2.0, an algorithm that utilizes a physics-based prior in concert with Bayesian optimization to efficiently search the material-space. We demonstrated the effectiveness of this method through closed-loop materials discovery with experimental collaborators. Based on known MPEA data, we used PAL 2.0 to recommend a list of high-hardness alloys, some of which the experimentalists then manufactured and tested. Using these results, we retrained PAL 2.0's models and derived new recommendations, thereby continuing the cycle. While our over 300-alloy dataset contained only four alloys with high hardness (hardness value > 1000), we were able to identify two more high-hardness alloys within just two feedback cycles. This shows that PAL 2.0 can greatly accelerate material discovery in a closed-loop approach. Currently, we hope to expand the search space with a clustering-based alloy generation algorithm to further identify novel, previously undiscovered alloy compositions.

Investigating Intrinsic Fluorescence Mechanisms in Amyloid Fibers

Aubrey Carey[1], Coral O'Brien[2], and Leah Spangler[*,1]
[1] Department of Chemical and Life Science Engineering, Virginia Commonwealth University
[2] Center for Pharmaceutical Engineering and Sciences, Virginia Commonwealth University

Fluorescent tags are minimally invasive fluorophore markers that can be used in live cells due to being largely non-toxic. For example, the artificial fluorescent tag Thioflavin T (ThT) is used for identifying amyloid fibers, protein aggregates that are often associated with diseases such as Parkinson's, Alzheimer's, and Type II Diabetes. Recently we have found that amyloid fibers have an intrinsic fluorescence that could be used as opposed to artificial dye like ThT. Here, we investigate this excitation-dependent fluorescence signal in fibers formed from Hen Egg White Lysozyme (HEWL). Batches of amyloid fibers were grown from HEWL with varying external conditions. We find that these lysozyme amyloid fibers have a previously unidentified absorbance peak at 350 nm separate from the UV signal given off by tryptophan at 280 nm. We also observe the excitation-dependent fluorescence from in the range of 420-500 nm with a Stokes shift of ~90 nm. By changing the growing conditions of the fibers, we have uncovered a potential correlation between fiber morphology and peak wavelength. With a better understanding of the correlation between fiber structure and their fluorescence pattern, it is possible that fluorescence can be used to identify proteins without the addition of dyes.

Abstracts - Poster Presentation

Coffee Off-Gassing Dynamics: Composition, Rate, with Corresponding Balances

Shane M. Coudriet[*,1], Katsuyuki Wakabayashi[1]
[1] Department of Chemical Engineering, Bucknell University, Lewisburg, PA

Nanocomposites have emerged as a promising area of research in recent decades due to their ability to improve the properties of host materials. Nanocomposites for cryogenic applications have gained significant attention for their potential in high-temperature superconducting (HTS) power transmission systems. However, exposure to low temperatures has detrimental effects on the mechanical properties of the material, limiting their applications. This necessitates the use of thermally stable high-quality dielectrics, which can be quantified through electrical and tensile testing. This paper discusses the preparation of poly(pyromellitic dianhydride-co-4,4'-oxydianiline), amic acid solution, and SiO_2 nanoparticles through a sol-gel process to create PA/SiO2 thin films. The team has performed a multitude of AC and DC dielectric tests and tensile tests at room temperature. The results of this research can help improve the understanding of these composites and their potential for use in cryogenic applications.

Membrane Reactor Applications for Methane and Water Production in Spacecraft Travel

Owen Gerdes[1], Vitor Gama[1], Oishi Sanyal[*,1], and Fernando Lima[*,1]
[1] Department of Chemical and Biomedical Engineering, West Virginia University, Morgantown, WV

As CO_2 levels rise, the concern surrounding its environmental impact highlights the increasing relevance with the Sabatier reaction. This reaction converts CO_2 and hydrogen into methane, which makes it effective for carbon utilization.
The Sabatier reaction has a unique application for on-board fuel generation using cabin air rich in CO_2. Intensified operations, like membrane reactors, may improve efficiency by increasing CO_2 conversion at equivalent temperatures, overcoming energy consumption challenges. The reactor is a shell and tube reactor, where cabin air is passed through the tube side, H_2 is passed through the shell side, and CO_2 passes through the membrane to the shell side, where the catalyst is packed, and the reaction can take place.
A membrane reactor and a traditional packed bed reactor (PBR) were simulated using AVEVA Process Simulation (APS). Each reactor carried out the Sabatier reaction and operated with equivalent space time. The two methods were assessed to compare the viability of the membrane reactor when compared with the common PBR. The respective conversions of the two reactors were made with the reactors operating at similar temperatures, H_2/CO_2 feed ratios, and catalyst amounts. Sensitivity analysis was then performed to find the ideal temperature range for the reactors.

Evaluating the effects of temperature on bacterial extracellular vesicle storages

Hayden Medlin[1], Ethan Bolinger[1], Robert D. Kirian[2], and Hannah C. Zierden[1,3]
[1] Chemical and Biomolecular Engineering Department 2. A. James Clark Department of Bioengineering, MD
[3] Department of Obstetrics, Gynecology, and Reproductive Sciences, University of Maryland College Park, MD

There are more bacterial cells in the human body than mammalian cells, and play a significant role in human health and disease. One mode of bacterial communication with host cells is via the production of bacterial extracellular vesicles (bEVs). bEVs are lipid-bound, nano-sized particles which carry small molecules, nucleic acids, and proteins to enable intraspecies and cross-kingdom communication. bEVs have inherent barrier-crossing and targeting capabilities, and emerging evidence of their contribution to human health and disease has garnered interest in using bEVs as drug delivery vehicles. This novel usage of biological nanoparticles as a therapeutic modality has great potential, but several manufacturing challenges must first be overcome. In particular, our current work is focused on the long-term storage of bEVs. We evaluated storage buffers and temperatures that best preserve bEVs for potential usage as drug delivery vehicles. By increasing longevity of bEVs by identifying optimal storage buffers, the potential for the translation of bEVs is dramatically improved. This foundational work is critical to revolutionizing the use of biological nanoparticles for therapeutic purposes.

Abstracts - Poster Presentation

Machine Learning Enabled Sustainability Assessment of New Chemicals and Processes

Milo Barkow[1], Mathew Conway[1], Jared Longo[2], John Pazik[1], Austin Lehr[1], Robert Hesketh[1], Kirti M. Yenkie[*,1]
[1] Department of Chemical Engineering, Rowan University, Glassboro, NJ
[1] Department of Mechanical Engineering, Rowan University, Glassboro, NJ

Life cycle assessment (LCA) is a systematic analysis of potential environmental impacts of raw materials, products, or services during their entire life cycle. Initial design stages are inherently complex and often lack comprehensive information, posing challenges for effective LCA evaluations. Machine Learning (ML) emerges as a valuable solution to address these challenges. ML algorithms, particularly Artificial Neural Networks (ANN), prove effective in predicting environmental impacts of new chemicals with limited data. This study focuses on comparing ML models trained on data sets consisting of a feature set (provided inputs) and a label set (predicted outputs). The feature set is comprised of both thermodynamic properties and molecular descriptors of the chemicals. The label dataset consisted of four endpoint and twelve midpoint impact assessment metrics. These assessment metrics are used in determining a chemical's impact on human health, resource utilization, ecosystem quality, and climate change. The effectiveness of the ANN algorithm was tested using a dataset of 500 points, divided into training, testing, and validation sets.

Phosphate recovery by Donnan dialysis: impact of operating parameters in a batch-recycle reactor

An Hong Dang[1], Sahar Souizi[1], and Lee Blaney[*,1]
[1] Chemical, Biochemical, and Environmental Engineering Department, University of Maryland, Baltimore County

New technologies are needed to address the grand challenge of nutrient pollution. We propose Donnan dialysis as a promising option for nutrient treatment and recovery. Donnan dialysis enables selective separation of nutrients across ion-exchange membranes due to electrochemical potential gradients induced by saline draw solutions. The objective of this study was to measure orthophosphate (P(V)) removal and recovery in lab-scale Donnan dialysis reactors designed to emulate continuous flow processes. Experiments were conducted in batch-recycle mode using two-chamber Donnan dialysis reactors equipped with anion-exchange membranes separating the nutrient-laden waste and saline draw solutions. The waste solution initially contained 10 mM NaH_2PO_4, and the draw solution was designed to achieve 90% recovery. The system was operated with variable mixing modes (with, without), volumetric flow rates (150, 300, 630 mL min–1), and waste-to-draw solution volume ratios (1:1, 3:1, 6:1). The optimal volumetric flow rate achieved almost 90% P(V) removal and over 87% P(V) recovery after 48 h. When the waste-to-draw solution volume ratio was changed from 1:1 to 6:1, the P(V) flux out of the waste solution increased by 30.2%, suggesting scale-up benefits. These outcomes highlight the potential of Donnan dialysis to be employed for effective nutrient recovery in continuous flow systems.

Crystallization Kinetics of Common Pharmaceuticals for Database Development

Kennedy Tomlinson[1], Joshua Zaharof[1], Ibrahim Joel[1], Kevin P. Girard[2], Alpana Thorat[2], Gerard Capellades[*,1]
[1] Department of Chemical Engineering, Rowan University, Glassboro, NJ
[2] Pfizer Worldwide Research and Development, Pfizer Inc., Groton, CT

Crystallization plays a crucial role in various industries, specifically pharmaceuticals, to purify or isolate a solid. This separation process has been used for years but there is a lack of knowledge on the molecular factors driving crystallization kinetics for nucleation and growth. The kinetic information for a specific system helps to give insight into a compound. Experimental methods in literature are not just time and material-intensive, but also strongly differ in scales, measurement approach, and choice of models.
A standard method of collecting crystallization kinetic data efficiently has been explored. This screening process is performed with a small amount of material, 1-4g, and can produce results in a few days. These systems undergo consistent experimental conditions that capture pictures of the crystals throughout the duration. The data extracted from experiments are implemented into a mathematical model to determine nucleation and growth constants. These constants for multiple different systems can be compiled in a database that contains crystallization kinetics. This process allows for a standardized workflow that produces results quickly. The database can aid process development by classifying a new system's kinetic behavior based on similar systems that were already analyzed. This method helps to advance and optimize the crystallization process.

Abstracts - Poster Presentation

Effect of Charge Modification on Peptide Penetration of Membrane

Abhiraman Senthilkumar[1], Dr. Jeffery B. Klauda[*,1]
[1] Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD

Cell-penetrating peptides (CPPs) can pass through the plasma membrane. Because of their antibiotic potential, the development of methods to enhance their cell-penetration ability is of significant interest. Model amphipathic peptide (MAP) is an artificial CPP that directly translocates through the cell membrane, causing damage in the process. MAP contains five positively-charged lysines, a key factor in its ability to cross the lipid bilayer. This project aims to develop mutants of MAP with higher penetration capability. Mutants with varying charges are generated by making single amino acid substitutions. These mutants are currently being computationally tested through molecular dynamics (MD) simulations with a bilayer designed to resemble C. albicans, using the Highly Mobile Membrane Mimetic (HMMM) model, which speeds up protein-membrane interactions. Mutants will then be synthesized and tested in vitro to verify results. Finally, a machine-learning model will be trained to generate novel mutants with improved penetration. This research will improve the current understanding of the effect of charge mutations on CPP translocation, and also be the first large MD analysis of MAP.

Effect of Anisotropic Incorporated Impurities on Crystal Growth and Dissolution

Abigail Martin[1], Joe Kratz[1], Claire Schleper[1], Gerard Capellades[*,1]
[1] Chemical Engineering, Rowan University, Glassboro, NJ

Thoroughly understanding solubility behavior is critical in the pharmaceutical industry, especially when it comes to effective and safe drug delivery. Drug manufacturing generally results in the production of small amounts of impurities in addition to the active pharmaceutical ingredient (API). These impurities are incorporated into the crystalline lattice of the API and are known to affect physical and chemical properties, most notably solubility and bioavailability. This research aimed to shed light on the effect of impurity incorporation on solubility. Due to its well-known behavior of region-specific impurity incorporation, a model system of potassium sulfate crystals with lattice incorporated acid fuchsin impurity was used to investigate crystal growth and dissolution. The dimensions of single, impure crystals with anisotropic lattice incorporated impurities were measured as they were aged in supersaturated and undersaturated solutions of potassium sulfate. It was observed that impure regions of the crystal experienced greater growth and dissolution rates compared to pure regions, proving that the impurity incorporation does affect spatial crystallization growth and dissolution behaviors. This understanding of the effects of impurity incorporation can be utilized in the drug manufacturing industry to minimize the adverse effects of impurities.

Synthesis of CeO2 Supported Period Four Transition Metal Catalysts via One Pot Chemical Vapor Deposition (OP-CVD) Method: Synthesis, Characterization, and Activity Test

William Chen[1], Hannah Karkout[1], Mary Calandra[1], Nicole Spencer[1], Amol Pophali[1], Ryuichi Shimogawa[1,2], Gihan Kwon[3], Anatoly Frenkel[1,2],Taejin Kim[*,1]
[1] Materials Science and Chemical Engineering Department, Stony Brook University
[2] Brookhaven National Laboratory
[3] National Synchrotron Light Source II, Brookhaven National Laboratory

Ceria supported catalysts play an important role in environmental and energy related fields because of its redox property. In this study, ceria supported MOx (M= Period four transition metals, such as Cr, Mn, Fe, Co, Ni, Cu, and Zn) catalysts were synthesized by one-pot chemical vapor deposition (OP-CVD) method. The physical properties of MOx/CeO2 including surface species dispersion on CeO2 and molecular structure were validated with thermogravimetric analysis (TGA), X-ray diffraction (XRD) spectroscopy, Raman spectroscopy, Inductively coupled plasma optical emission spectrometry (ICP-OES), and scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM/EDX). The characterization results confirmed that surface transition metal oxides were effectively dispersed and adsorbed on CeO2. The synthesized catalysts were applied to the CO oxidation reaction as a model reaction. Among the catalysts, CuO/CeO2 showed the highest catalytic activity (~98% CO conversion at ~155 °C). The obtained result provided the feasibility of OP CVD method to synthesize a different type of supported catalysts effectively: no solvent, and relatively simple synthesis procedures (solid-mixing, evaporation, and calcination). The synthesized supported catalysts can be applied to broad ranges of catalysis areas.

Abstracts - Poster Presentation

SEA Metal Loading of a Novel Catalyst

Connor Richeson[1,2], Dr. Frank Gupton.[*,1]
[1] Department of Chemical and Life Science Engineering, Center for Rational Catalyst Synthesis

The rise in heterogeneous catalysts can be derived from the innate problems associated with their pure counterparts, homogeneous catalysts. Homogeneous catalysts rely solely on the active metal to complete the reaction, however, removing the catalyst from the solution or solid can be far more difficult than it is worth. Despite this, platinum group metals are some of the most expensive in the available market. Heterogeneous catalysts, in comparison, are bound to a support which makes the metal far easier to extract after a reaction and can act as a potential assistant to the metal. The specific structure this project aimed to refine uses a carbon-alumina based structure to support the platinum group metal. The supports were longitudinally analyzed as candidates for SEA uptake using pH shift techniques and Inductively Coupled Plasma Optical Emission spectroscopy to measure metallic concentrations. Effectivity was measured with a standard cross-coupling reaction. GCMS supported that the reaction did not complete. The supports and reduced metals were found to be unsuccessful, likely showing unpredicted bonding to the support's surface.

Computational Analysis of N2 Reduction to NH3 using a Mo-I Based Catalyst

Ryan C. Zmarzlak[1], Yan Choi Lam[1]
[1] Department of Chemistry, Bucknell University

The Haber-Bosch Process is an industrial process that affects the lives of nearly everyone on Earth as 14 million metric tonnes of Ammonia produced per year provide farmers with fertilizer to efficiently feed most of the world's population. However, the process produces 500 million tons of CO_2 emissions per year as a byproduct. By using a weak acid in Collidinium Triflate, a reductant in Decamethylcobaltocene, which is then paired with a Nitrogen gas in a Toluene solvent, Ammonia will be produced without creating Carbon Dioxide. An Mo-I based Catalyst will ensure Ammonia is produced by a complex PCET (Proton Charge Electron Transfer) catalytic cycle efficiently at room temperature. The goal behind this process was to study this catalytic cycle in creating Ammonia for its thermodynamics and Gibbs Free Energy to ensure that Ammonia was not only produced, but also optimally produced in large quantities when compared to today's production of Ammonia in various chemical plants around the world. Computer simulations were completed in software to complete this task as various optimization steps such as limiting and understanding ion-dipole interactions between the acid and catalyst. Another step taken is changing the organic structure of the Mo-I based Catalyst.

Role of Extracellular Vesicles (EVs) as Biomarkers for Preeclampisa

Yasmi Chibber[1], Hannah C. Zierden[1,2,3], Yasmi Chibber[*,1]
[1] Department of Chemical & Biomolecular Engineering, University of Maryland
[2] Fischell Department of Bioengineering, University of Maryland
[3] Department of Obstetrics, Gynecology and Reproductive Sciences, University of Maryland School of Medicine

Preeclampsia is the leading cause of deaths in mothers and fetuses worldwide. A disease in which the placenta becomes inflamed, preeclampsia affects nearly 1 in 10 pregnancies and manifests as high blood pressure. The only known cure to the disease is to induce labor, often leading to a premature delivery. Beyond the adverse neonatal impacts, mothers are at risk for stroke, organ failure, and/or blood-clotting disorders. Many day-to-day symptoms of preeclampsia mirror those of a healthy pregnancy, creating a critical need to identify a biomarker of preeclampsia to develop better treatment options, and improve health outcomes. We hypothesized that extracellular vesicles (EVs) may serve as an early detection mechanism. EVs are lipid-bound nanoparticles produced by all cells that carry biological cargoes reflective of the parent cell. During pregnancy, EVs produced by the placenta may be used to determine placental function. Plasma samples from healthy and preeclamptic mothers were collected. EVs were isolated using size exclusion chromatography and were characterized using nanoparticle tracking analysis. We identified differences in the concentration, size, and surface charge of EVs, which may alter cellular signaling during pregnancy. This work has important implications for improving outcomes for women with preeclampsia by improving earlier detection capabilities.

Abstracts - Poster Presentation

Exploring Machine Learning Models for Predicting Vapor Pressure

Elijah Kaplowitz[1], Charles McGill[*,1]
[1] Department of Chemical and Life Science Engineering, Virginia Commonwealth University

The current methodology of vapor pressure relies on empirical equations like Antoine's equation, which require experimental coefficients for each molecule and temperature range, limiting the ability to extrapolate to new species and wider temperature ranges. This study aims to develop a machine learning model using Chemprop to predict vapor pressure. In this study, we explore various model structures, which include: a basic model directly predicting pressure from training data with temperature as a feature, a more complex model predicting Antoine coefficients first, and a method introducing noise to temperature to prevent overfitting. Vapor pressure data from DIPPR is utilized to train these models. We evaluate the impact of different structures on model accuracy and discuss potential combinations for optimal performance, considering scenarios with limited data availability and extrapolation beyond fitted ranges. Additionally, future considerations involve incorporating predictions of critical temperature and pressure as extra features, as well as incorporating uncertainty prediction into these model structures.

Enhancing Wound Healing Through Allographic Skin Grafts and Tissue Engineering: A Multifaceted Approach to Promote Angiogenesis, Mitigate Graft Rejection, and Scale Production

Briman Yang[1], Shi Fu[1], Huiting Luo[1], Kuan-Che Fang[1], Marcia Simons[2], Miriam Rafailovich[1], Gurtej Singh[3]
[1] Department Chemical and Molecular Engineering and Material Science, Stony Brook University
[2] Department of Oral Biology and Pathology, Stony Brook University
[3] Department of Surgery, Stony Brook University

This research proposal presents a novel strategy to enhance wound healing and tissue engineering processes, specifically targeting the crucial stages of proliferation and remodeling. The study introduces an advanced approach in the development of allographic skin grafts by integrating scaffold materials and biologically active molecules, aiming to improve graft functionality and encourage angiogenesis within the skin constructs. The research employs a comprehensive multidisciplinary methodology, leveraging dental pulp stem cells, human umbilical vein endothelial cells (HUVECs), fibroblasts, and a collagen matrix to replicate the intricate biological conditions essential for efficient wound recovery. Innovations include experimenting with titanium dioxide nanoparticles to assess their impact on HUVEC network formation and employing supercritical CO2 for the decellularization of skin constructs. By tackling prevalent issues in both autologous and allograft skin grafting, such as graft rejection and production scalability, this project aims to make significant contributions towards scaffold fabrication and vasculature improvement. Ultimately, this research endeavors to advance the field of tissue engineering, opening up new pathways for treating extensive surface wounds and burns, thereby enhancing the quality of life and care for patients afflicted with severe skin injuries.

Exploring Laurdan's Fluorescence in a Ternary System of DOPC, DSPC, & Cholesterol

Riley Szumachowski[1], Thomas Kinard[1], and Steven Wrenn[*,1]
[1] Department of Chemical Engineering, Virginia Tech

The ternary lipid system of 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC), 1,2-distearoyl-sn-glycero-3-phosphocholine (DSPC), and cholesterol is the subject of our study. This system has been shown to contain three distinct membrane phases, as well as coexistence between them. Our investigation utilizes a trio of fluorescence techniques to investigate lipid bilayer mechanics as a function of composition. The fluorophore employed in all three techniques is Laurdan, a sensitive probe for monitoring lipid membrane organization. First, Laurdan's emission exhibits a spectral shift in response to changes in the polarity of the lipid environment, which is commonly quantified as "Generalized Polarization" (GP). Fluorescence anisotropy and lifetime are the remaining two techniques, which serve to quantify the fluidity of the probe environment. The results of all three techniques used are compared.
Our research may provide insight into the transition and coexistence between the different lipid phases that occur within the bilayer. Implementation of Laurdan in these assays not only enhances our understanding of the dynamics of bilayers consisting of DOPC/DSPC/Cholesterol, but also offers valuable insights into membrane biophysics more broadly. The findings have the potential to have implications in various fields, including pharmaceuticals, medicine, and biotechnology, where an in-depth and thorough understanding of lipid membrane properties is critical.

Abstracts - Poster Presentation

Thermo-mechanical Property for 3D printed Carbon-Fiber Reinforced Polyamide Composite.

Rwaka Bruce Furaha[1,2], Martin Etemadi[1,2], Justin Anderson[1,2] and Michael Bortner[*,1,2]
[1] Department of Chemical Engineering, Virginia Tech, Blacksburg, VA
[2] Macromolecules Innovation Institute, Virginia Tech, Blacksburg, VA

Carbon fiber reinforced composites are known for their stiffness and high specific strength. Current advancement in additive manufacturing enables 3d printed CFRPs with a controlled variation of fiber content and fiber directionality. However, the mechanical properties of 3D printed CFRPs exhibit high variability when compared to conventional CFRP fabrication approaches. As part of an effort to build a predictive model for thermo-mechanical properties of 3D printed CFRPs, this poster discusses the results obtained in the study of 3D printed carbon fiber reinforced nylon (CFRPs) parts with varying fiber content and fiber directionality. Samples were printed on a Markforged printer using 3 raster angles of 0,45-, and 90-degree angle. The fiber content was varied by changing the number of carbon fiber layers in samples. The printed samples were then evaluated using Dynamic Mechanical Analysis (DMA) and Differential Scanning Calorimetry (DSC). The results suggest that thermo-mechanical analysis can be used to predict and optimize the design of 3d printed CFRPs.

Developing Mechanistic Understanding of Zinc Plating vs Zinc-ion Intercalation in Chevrel-phase Mo6Se8

Sara Avraham[1], Tricia M. Marchese[1], Brian Chen[1], Robert J. Messinger[*,1]
[1] Department of Chemical Engineering, The City College of New York, CUNY, New York, NY

In this work, we studied the interplay between Zn2+ intercalation and Zn plating in chevrel-phase Mo6Se8 cathodes for Zn-ion batteries. We demonstrated for the first time that Zn can plate on Mo6Se8 cathodes in Zn/Mo6Se8 cells; Zn deposits were evidenced using optical microscopy, scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy, and X-ray diffraction on galvanostatically discharged Mo6Se8electrodes. Zn plating was further investigated through galvanostatic measurement of the plating overpotential, which appears as a minimum in the Zn/Mo6Se8 cell potential during discharge below 0 V. Variable-temperature (-10~+60 °C) and variable-current (10~1000 mA/g) measurements of the plating overpotential revealed an interplay between Zn2+ intercalation, the hydrogen evolution reaction, and Zn plating on the Mo6Se8 electrode surface. An Arrhenius analysis for temperature-dependent Zn plating overpotentials at 10 mA/g showed that the Zn plating process possessed a negative apparent activation energy of -9.41 kJ/mol, which is indicative of a multi-step plating mechanism and reveals the significance of ion adsorption on the electrochemical kinetics of Zn plating. Furthermore, SEM images on galvanostatically discharged Mo6Se8 electrodes (10 mA/g) at -10, +20, and +60 °C showed the formation of Zn deposits that assumed hexagonal morphology of either thin (-10 °C) or thick (+60 °C) plates.

Optimizing process parameters for preparation of biodegradable polymer nanoparticles using flash nanocomplexation and nanoprecipitation methods

Sachin V. Kammula[1,2], Yuanmuhuang Long[2,3], Yicheng Zhang[2,4], and Hai-Quan Mao[*,2,3,4]
[1] Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD
[2] Institute for NanoBioTechnology, Johns Hopkins University, Baltimore, MD
[3] Department of Biomedical Engineering, Johns Hopkins University, Baltimore, MD
[4] Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, MD

Developing scalable, reproducible, and efficient protocols for polymeric nanoparticle (NP) manufacturing remains a challenge in nanomedicine. The combined flash nanocomplexation (FNC)/flash nanoprecipitation (FNP) process has been developed to enable rapid and uniform assembly of nanoparticles with high payload capacity. This study examined the effects of polymer solvent and key processing conditions (flow rates, purification strategy) on nanoparticle size/uniformity, drug-loading efficiency, and release rate, using a multi-inlet vortex mixer setup with doxorubicin (DOX) and immunoglobulin G (IgG) as surrogate payloads. DOX was loaded into the nanoparticles using a hydrogen-bonding-mediated FNC/FNP formulation method; four water-miscible solvents were tested at high flow rates and produced uniform DOX-loaded NPs with consistent drug encapsulation (~80-90 percent) and tunable loading. NPs prepared with DMSO showed a superior sustained release (14-day vs. < seven-day) and high stability, with denser polymeric packing. Applying this testing pipeline for electrostatics-mediated FNC/FNP-formulated particles indicated superior stability and release for IgG NPs produced using acetonitrile as a solvent. Solvent selection and mixing conditions modulate NP assembly and delivery efficiency and are dependent on FNC secondary interactions/encapsulation strategy. This study enhances understanding of microfluidic-driven NP assembly to tune drug release, while also validating a high-throughput purification method enabling industrial scale-up.

Abstracts - Poster Presentation

Discovering Equations for Simple Acids Dissociation

Fariha Agbere[1], Samiha Sharlin[1], Kianoush Ramezani Shabolaghi[1], Tyler R. Josephson[*,1]
[1] Department of Chemical, Biochemical and Environmental Engineering,

Zeolites are versatile microporous crystals widely used as valuable adsorbents in various industries, thanks to their unique TO4 building block, primarily silicon (Si). Brønsted acid zeolites, formed by the replacement of Si by elements like aluminum (Al) or phosphorus (P), exhibit acid functionality, enhancing their catalytic and adsorptive capabilities. We aim to study interactions in zeolite adsorption, particularly in Brønsted acid zeolites, but we face challenges in finding affordable and reliable methods. While Density Functional Theory (DFT) offers accuracy, it's costly for large-scale systems. In contrast, molecular mechanics force fields are available for simulations, but they have not been well-established for studying acid-base interactions in Brønsted acid zeolites. To address this, we're developing transferable force fields tailored for acid-base interactions with the help of symbolic regression, which allows us to derive functional forms of interaction potentials from potential energy surface scan data. Our methodology and findings will primarily focus on simple systems such as HCl, HF, and HBr, illustrating how symbolic regression could potentially facilitate bridging the gap between accurate yet expensive DFT calculations and more accessible force field simulations.

Bimetallic Complexes for Alkyne Trimerization

Alexander Davis[1,2], Matthew Williams[1], and Diana Thornton[*,1]
[1] Department of Chemistry, Virginia Tech, Blacksburg, 24060

The goal of this project is to synthesize first-row transition metal complex pairs capable of selectively cleaving strong bonds, such as C-H bonds. The importance of this lies in the global demand for more sustainable production methods without the need for extreme reaction conditions or reliance on noble metal catalysts. We hypothesize that using weak field ligands, such as alkoxides, will allow for high spin electron configurations in first-row metal centers, increasing their reactivity. Using an alkoxide-based ligand, mononuclear vanadium and cobalt complexes have been identified. Testing for metal-metal cooperativity, we found that the vanadium/cobalt pair promotes the trimerization of alkynes under mild temperatures. The cobalt complex, when used individually, catalyzes the reaction of aryl acetylenes to yield a 1,2,4-substituted benzene isomer when initiated with excess alkynes, ultimately achieving full consumption of the reagent. However, when using the cobalt and vanadium complexes together the reaction selectively produces the 1,3,5-substituted benzene isomer without the need for excess alkynes to initiate the reaction. We monitor reactions via 1H and 31P NMR and GC-MS to evaluate reaction selectivity and progression. Moreover, we also seek to crystallize reactive intermediates to identify the reaction mechanism and understand the metal-metal cooperativity.

Stimulating Collateral Arterial Growth Using Acellular, Growth-Factor Free Hydrogels for the Treatment of Critical Limb Ischemia

Raey Hunde[1], Corinne Curry[2], Nicole Marguerite[2], Akhila Ramgiri[2], Mukesh Gupta[3], and Ethan Lippmann*[2]
[1] Chemical, Biochemical, and Environmental Engineering, University of Maryland, Baltimore County
[2] Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN
[3] Biomedical Engineering, Vanderbilt University, Nashville, TN

Critical Limb Ischemia (CLI), a severe manifestation of Peripheral Artery Disease (PAD), involves a significant blockage in the lower extremity arteries, causing a pronounced reduction in blood flow, especially in diabetic or chronic smoker patients. This diminished blood supply leads to tissue necrosis, often necessitating amputation. The current lack of robust treatment options for CLI has resulted in unsuccessful clinical trials attempting to stimulate arterial growth through growth-factor encapsulated hydrogels. Our proposed alternative method focuses on utilizing acellular, growth factor-free hydrogels to induce arteriogenesis. This involves two main steps: (1) advancing the development and characterization of the GelCad hydrogel (gelatin-based with attached Cadherin peptides), synthesizing it into microspheres, and (2) implementing a cell-responsive siRNA release strategy to trigger arteriogenesis via macrophage polarization. Promising preliminary results demonstrate the synthesis of GelCad microspheres using 3,3'-Dithiodipropionic acid di(N-hydroxysuccinimide ester), a reactive oxygen species (ROS) capable of macrophage polarization. This proposal aims to create a potent GelCad hydrogel suitable for clinical use, potentially revolutionizing the treatment of PAD. The success of this innovative strategy could significantly enhance blood flow, contributing to the reversal or prevention of tissue ischemia in patients with CLI.

Abstracts - Poster Presentation

Relationship Between Grind Size, Shape, Surface Area, and Coffee Quality Degradation

Maya A. Fetzer*,[1] and Katsuyuki Wakabayashi[1]
[1] Department of Chemical Engineering, Bucknell University, Lewisburg, PA

The coffee industry placed enormous emphasis on the freshness of the beans and grounds used to make brewed coffee. This research correlated how trends between size, shape, and surface area of ground coffee varied based on well-controlled operational factors such as storing condition and time since initial roast. Brazil Cerrado coffee beans were roasted in-house to the darkness of City+ (-13.4% weight loss) and ground at varying times since the green beans were initially roasted. Coffee beans were stored in four air-tight containers placed in ambient room conditions, most conditions (RH>80%), dry conditions (RH<15%), and a freezer. These conditions were chosen because of their prevalence as storing conditions in the coffee industry. A Camsizer X2 Dry was used to analyze samples of coffee grinds for the distribution of size, symmetry, and sphericity. The collected data revealed trends between the change in size and shape of the coffee grounds as time passed based on the temperature and moisture of the storage conditions. Understanding how size, shape, and surface area of ground coffee varied in response to operational factors allowed for better quality control and optimization of the brewing process.

Surfactant Inhibition of Cuprous Oxide Antimicrobial Activity

Summer Hensley[1], Thomas Brown[1], Bri Tran[1], Zach Benmamoun[1], and William Ducker*,[1]
[1]Department of Chemical Engineering, Virginia Tech, Blacksburg, VA

Cuprous oxide is a well-known antimicrobial agent. Here we examined how the efficacy of cuprous oxide is affected by the presence of surfactants. This is important because surfactants are commonly used in cleaning products and in some antimicrobial formulations and care should be taken so as not to inactivate the antimicrobial. Surfactants investigated were sodium dodecyl sulfate (often used in detergents), Tween-20, and rhamnolipid, a biosurfactant produced by the bacterium, pseudomonas aeruginosa. Upon combining bacteria, cuprous oxide, and surfactant, below, at, and above their respective critical micelle concentration, the colony-forming assay was performed to determine bacterial viability. Strain (gram-positive and -negative), contact time, and order of addition were not significant factors. Tween-20 and rhamnolipids inhibited cuprous oxide's killing ability; SDS did not. Results were analyzed as log comparisons between the control (surfactant alone) and surfactant with cuprous, to isolate the effect of cuprous oxide. SDS and cuprous oxide are both negatively charged. The zeta potential of E. coli was found to be negative as well. However, SDS was found to bind to cuprous oxide, therefore the results cannot be explained by only charge repulsion. We conclude the effect of surfactants on cuprous oxide efficacy depends on the surfactant

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Optimization of Chitosan-Based Electrolytes for Zn-ion Batteries

Nathaniel Glover[1,2], Usman Ali Khan[1], and Deepa Madan*,[1]
[1]Mechanical engineering, University of Maryland, Baltimore County, Baltimore, MD
[2]Chemical engineering, University of Maryland, Baltimore County, Baltimore, MD

While lithium currently acts as our primary source for rechargeable batteries, concerns with its environmental harm and hazardous properties give cause to search for sustainable alternatives for energy storage. Zinc-ion batteries provide an exciting avenue for a safe and eco-friendly alternative to lithium-ion batteries. However, two primary challenges prevent Zn-ion batteries from being reliable energy storage devices. One is the lack of an optimal electrolyte and the other is dendrite formation from the zinc anode reducing the recyclability of the batteries. This project sought to address these challenges with the development of a densified chitosan-based electrolyte. These electrolytes are made from polyvinyl-alcohol (PVA) which absorbs Potassium Hydroxide (KOH), the active reagent in the electrochemical reaction that takes place within the battery, with chitosan acting as a binding agent. Our team tested a series of compositions of chitosan and PVA to maximize ionic conductivity, producing more effective electrolytes. Additionally, to improve the recyclability of our batteries, we sought to test the efficacy of adding Zn(OTF)2 to our electrolyte solution. Our results show a promising trend that will allow us to develop optimal electrolytes with consistently high ionic conductivities while improving the recyclability of Zn-Mg batteries.

Abstracts - Poster Presentation

Enhancing Engineering Education Through Pilot Plant Development

Emma Padros[1], David Theuma[1] , Michael Fracciolla[1], Steven Roth[1], Barnabas Gao[1], Kirti M. Yenkie[*,1], Robert P. Hesketh[*,1], C. Stewart Slater[*,1]

[1] Department of Chemical Engineering, Rowan University, Glassboro NJ

Students developed and implemented a laboratory scale pilot plant to optimize the flushing process during product changeovers in lube oil processing facilities. The existing flushing process has operational inefficiencies which leads to product contamination. Thus, the goal of this project was to understand these inefficiencies and use engineering concepts to enhance this process using a pilot plant. The pilot plant, a one-to-five scale down of an industrial packaging plant, enabled a detailed study of lube oil properties, pipeline dynamics, filter types, and flushing techniques by matching industry conditions. Students engaged in adjusting oil flow rates via a positive displacement pump and utilized an inline viscometer to determine oil product purity. The pilot plant can help identify when the flushing process is complete and optimize flushing volume and minimize oil downgrade. Students conducted and analyzed residence time distributions on the pilot plant flushes using data analysis software. This confirms the pilot plant's accuracy in mimicking industrial process conditions and in optimizing flush volume. This study serves as a data source for industrial application and as an educational tool, providing students with essential skills for engineering practice and preparing them to face real life engineering challenges.

Verification of Hemostatic Nanocapsules Through Property Characterization and Their Clotting Strength Through Rotational Thromboelastometry Analysis

Chiad Onyeje[1] , Aye Tuedon[1] , and Erin Lavik[*,1]

[1] Chemical, Biochemical, and Environmental Engineering, University of Maryland, Baltimore County

Trauma-induced bleeding can be beneficially impacted by blood clot formation, though few methods currently exist to increase the clotting rate for internal first aid. Bleeding is a leading cause of preventable, post-injury death; with recent innovations in therapeutics, there is a keen focus on such preventability. As such, we have produced polymer-based hemostatic nanocapsules as drug delivery vehicles that intravenously induce blood clots within injury models—and are a potential method of trauma aid. Synthesized as polyurethane shells from a polymerization emulsion, the nanomaterial is conjugated with a peptide moiety (GRGDS) which targets and initiates clotting in activated platelets during hemorrhage. Through rigorous characterizations, these nanocapsules have shown sizing and charge acute to the expected bio-environment, as well as successful peptide conjugations through PEG linkages between the shell and conjugate. The current research tested nanocapsule hemostatic strength through rotational thromboelastometry (ROTEM) machinery, working to accelerate clot formation time in a monitored, in-vitro modality. For this phase, anticoagulant Heparin was drug-loaded to showcase evidence of clotting-unclotting control of the nanocapsule, both essential to assuring patient safety. As we continue ROTEM testing, our coming results perceive finely controlled clotting nano-biomaterials capable of acting as internal bandages.

Developing an Online ATP Sensor for Cell-free Protein Synthesis

Elias Gilotte[1], Chad Sundberg[1], Hasib Hasan[2], Govind Rao[1]

[1] Department of Chemical, Biological, and Environmental Engineering, University of Maryland Baltimore County

[2] Department of Computer Science and Electrical Engineering, University of Maryland Baltimore County

A barrier to cell-free protein synthesis (CFPS) scale-up is the lack of options for process monitoring of energy substrates. CFPS has the potential to replace live-cell bioreactors for rapid, large-scale manufacturing of biologics. A vital substrate is adenosine triphosphate (ATP) because it is the energy currency in CFPS. Existing ATP quantification methods are resource-intensive making them impractical for continuous ATP monitoring. To address this challenge, we designed a low-cost sensor, ≈$15 per chip for online, automated ATP monitoring. The recognition element is a fluorescent protein that selectively binds ATP, leading to changes in fluorescence intensity upon ATP binding. The protein is immobilized in a microfluidic chip and interfaced with the Center for Advanced Sensor Technology's proprietary biochemical analyzer, an adaptable platform for collecting and processing signal data. One microfluidic chip can be used for 20 consecutive samples at a maximum rate of one sample every 10 minutes. The ATP sensor's broad detection range of 150 uM to 10 mM ATP was validated by comparison with a standard luciferase based ATP assay. Continuous ATP monitoring could enable further CFPS process development efforts to improve reaction longevity and product yields.

Abstracts - Poster Presentation

Characterizing the Aspergillus nidulans Kinase Deletion Library for Differential Septation in Response to Cell Wall Stress

Meredith Morse[1], Joshua Dayie1, Feonil G. Limiac[2], Raina B. Miller[3], Rianna S. Minter[4], Greeshma Tarimala[5], Mael Ndlamba[6], Shavier Small[7], Alexander Doan[1], Mark R. Marten[1]
[1] UMBC, Department of Chemical, Biochemical, and Environmental Engineering, Baltimore, MD
[2] Towson University, Department of Molecular Biology, Biochemistry, and Bioinformatics (MBBB)
[3] Southern Nazarene University, Department of Biology-Chemistry
[4] Delaware State University, Department of Biological Sciences
[5] Mount Hebron High School, Applications and Research Laboratory
[6] Biochemistry, Loyola University Maryland
[7] Chemical and Biomolecular Engineering, Johns Hopkins University

Filamentous fungi employ complex signaling pathways to regulate cell-wall integrity and repair, predominantly mediated by protein kinases. However, many of the 98 nonessential protein kinases in the model fungus Aspergillus nidulans are uncharacterized. Previous research in our lab has shown septation is important for surviving cell wall stress. By determining which kinases are involved in septation, we can generate targets for more effective antifungal drugs that inhibit septation. Antifungal drugs that deplete the response to cell wall stress are essential for treating patients with fungal infections. For this purpose, various strains were grown from the A. nidulans kinase deletion library, each lacking one specific kinase gene. To test the hypothesis that certain kinases are involved in responding to cell-wall stress, the library strains were grown for 16 hours under two conditions: with and without micafungin, a cell-wall perturbant triggering septation. Fluorescent microscopy captured images of the fungal cells, which were analyzed for extent of growth and number of septa formed. By comparing the phenotypes of the mutant strains to an isogenic control strain, the involvement of the various kinases in responding to wall stress can be inferred.

A Machine-Learning Approach to Simulate Confined Liquid Lithium Polysulfides for Battery Applications

Joshua Zhou [1,2], Brandon Bukowski[*,1]
[1] Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD

While lithium-sulfur batteries have great potential to be an environmentally friendly alternative to existing lithium-ion batteries, the battery loses effective mass during cycling due to the transport of liquid polysulfides to the cathode. It has been shown that embedding a metal-organic framework (MOF), a porous material, can dramatically improve the battery's cycling capabilities by reducing polysulfide diffusion. However, the underlying mechanisms are not yet well understood. Here, we investigate how lithium and sulfur interact as a confined liquid. Our simulations use the extended Tight Binding (GFN-xTB) semi-empirical methods. We also use Parinello meta-dynamics to sample a wider area in chemical configuration space. The energy, force, and coordinate data generated from these molecular simulations were used to train a machine-learning model using DeePMD. This model is then used to simulate a lithium-sulfur-MOF system with an order of magnitude more atoms than can be conventionally done using strictly ab initio techniques. We intend to integrate other compounds, such as solvents and battery nodes, into our simulations. We hope to understand why lithium and sulfur atoms interact differently in the presence of a MOF, what features of these MOFs best suit our needs, and how we may best utilize them.

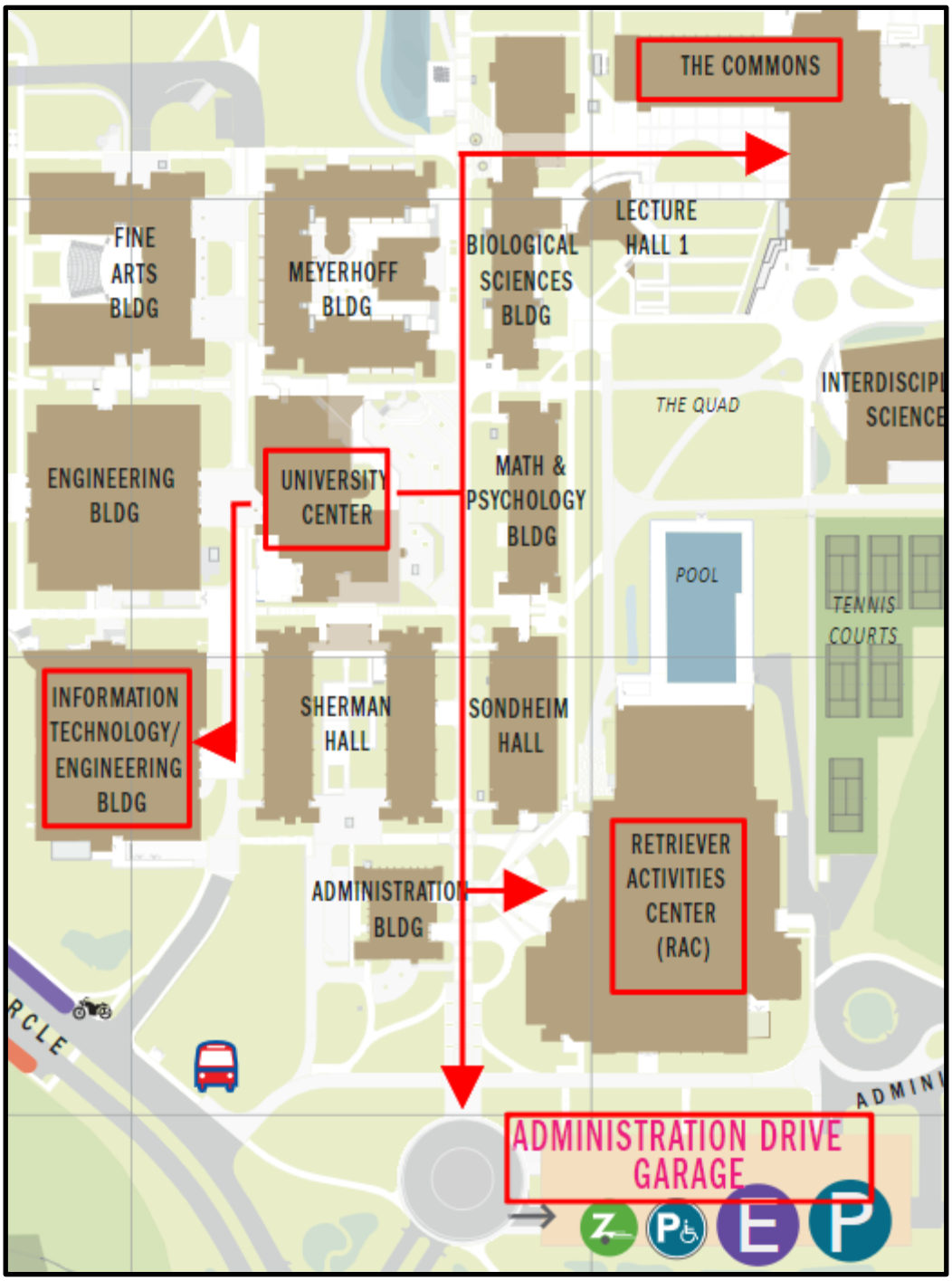
Optimized Expression of an Antimicrobial Peptide in the Yeast Surface Display System

Natalya Brown[1], Wright Makambi[1], and Amy Karlsson[*,1]
[1] Chemical and Biomolecular Engineering, University of Maryland, College Park

Candida albicans, an opportunistic fungal pathogen in the oral cavity, often leads to infections like oral candidiasis. Despite the antifungal efficacy of salivary peptide Histatin 5 (Hst5) against C. albicans, its vulnerability to proteolysis by the C. albicans' secreted aspartyl proteases (Saps) limits its effectiveness. Addressing this, our lab previously identified more stable Hst5 variants using mass spectrometry and gel electrophoresis, but found the screening process lengthy and inefficient. In an effort to optimize this screening, we employed yeast surface displays on Saccharomyces cerevisiae (EBY100) for high-throughput screening of Hst5 variants, assessing their proteolytic stability. This involved optimizing expression conditions by adjusting temperature, pH, and buffer composition, and utilizing western blotting and flow cytometry to quantify expression and degradation. Our findings demonstrate that Hst5 can be quantifiably expressed on yeast cell surfaces, facilitating the efficient screening of mutant libraries for Sap resistance. This research holds promise for developing robust antifungal agents, significantly impacting public health by improving treatments for fungal infections.

Campus Map & Directions

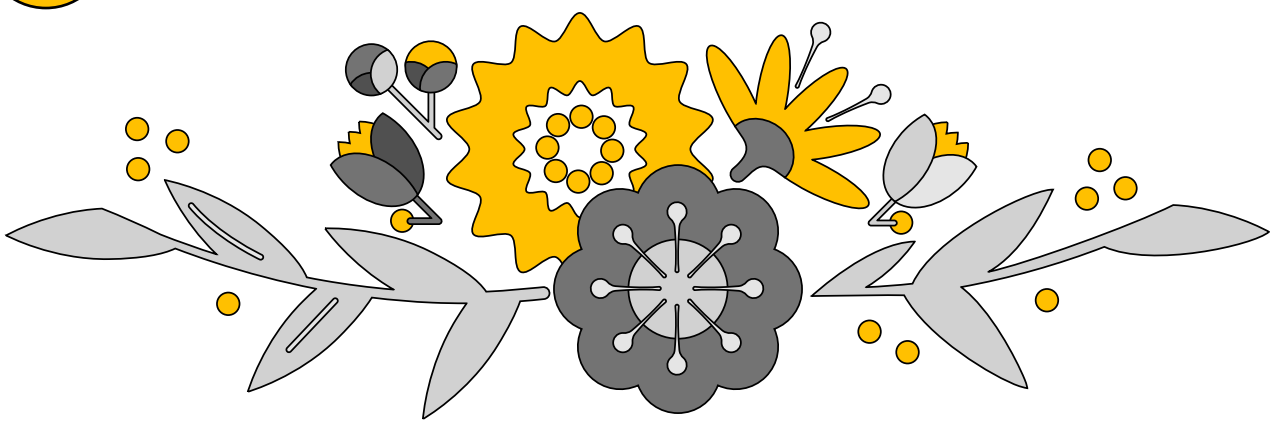
For detailed parking and campus directions, check out our **website!**



UC: University Center
ITE: Information Technology and Engineering building
RAC: Retriever Activities Center

Acknowledgement

We would like to acknowledge all our **sponsors, GritStarter donors, student volunteers, faculty and industry judges, and attendees from all participating institutions** for making this conference possible!



Thank you for your participation!