Presentation Number: 200

Presentation Title: Molecular Modeling and Simulation of 3-Hydroxybutyric Acid in Aqueous, Ionic Liquid, and Deep Eutectic Solutions

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Advisor: Dr. Ken Benjamin
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Abstract: 3-Hydroxybutyric acid (3HBA) is an important biosynthetic intermediate and biopolymer precursor. Although prior modeling has focused on biomedical derivatives, its behavior in biopolymer and bioprocessing contexts remains unexplored.

This work combines molecular dynamics and quantum chemical methods to investigate the liquid-phase thermodynamic and structural behavior of 3HBA in water, synthetic ionic liquids, and deep eutectic solvents. In aqueous systems, 3HBA is modeled with the CHARMM36 force field and water with TIP3P. Electrostatic point charges for 3HBA were derived using the CHELPG method at the CBS-Q3 level of theory. All-atom simulations were performed to analyze mixture properties and intermolecular interactions, including 3HBA–3HBA, 3HBA–water, and water–water aggregation.

COSMO-based quantum chemical calculations using COSMOtherm were also conducted to determine infinite dilution activity coefficients of 3HBA in water and alternative solvents. These results inform the selection of greener solvents for 3HBA extraction in bioprocessing applications.

Oral Presentation
Undergraduate Student

Presentation Number: 201
Presentation Title: Physical Separation and Characterization of Micrometeorites from Belle Fourche Shale

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Abstract: The Earth is continually showered with micrometeorites (MMs). In this study MMs were collected in fossilized form from Belle Fourche Shale (BFS). BFS was comminuted (hammer mill) to liberate individual particles, slurried, and separated into magnetic/non-magnetic fractions using wet high intensity magnetic separation (WHIMS). The magnetic particles were classified by size, and a stereomicroscope was used to identify (based upon sphericity) potential MMs. This physical separation resulted in a flux of 40 MM prospects in 26.4 kg of BFS. Potential MMs were next analyzed with a scanning electron microscope (SEM). The SEM allowed high resolution and imaging as well as energy dispersive x-ray spectroscopy (EDS). Further characterization of potential MMs was performed using a focused ion beam (FIB) and a transmission electron microscope (TEM). EDS revealed that many of the MM prospects were composed of iron oxides (magnetite (Fe_3O_4) and wustite (FeO)) as well as iron silicates like olivine $(Mg, Fe)_2SiO_4$. Tungsten and tantalum-nickel based particles were also found, however further analysis of these prospects is needed to confirm their origin (anthropogenic or not).

Oral Presentation
Undergraduate Student

Presentation Number: 202
Presentation Title: MPS Microenvironment Characterization For Further Study Of Ovarian Cancer

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Advisor: Dr. Travis W. Walker
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Abstract: Ovarian cancer is the 5th-leading cause of death among women in developed countries, with a 5-year survival rate of only 15%. Nearly 80% of cases develop chemotherapeutic resistance, yet 95% of novel chemotherapeutics fail in clinical trials. These failures are largely due to inadequate preclinical models. Current approaches rely on simplistic 2D cell culture, microfluidics, and animal models, which fail to sufficiently recapitulate human physiology. Micro-physiological systems (MPS) represent a promising next generation of advanced in vitro models that are capable of better mimicking a tumor microenvironment. This project aims to characterize the microenvironment for an MPS that is designed for the further study of ovarian cancer. Central to developing a representative MPS is matching the mechanical properties of the native ovarian microenvironment. Stiffness is a critical regulator of cell differentiation, motility, and adaptability. To this end, we quantify the stiffness of collagen hydrogels across varying construction parameters, including collagen concentration and crosslinking conditions. A combination of compressional and shear rheology is employed to establish the relationship between these parameters and the resulting mechanical properties.

Oral Presentation
Undergraduate Student

Presentation Number: 203
Presentation Title: Simulation Study for Improving Current X-Ray Medical Diagnostics with New Gamma-Ray High-Purity Germanium Detectors

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Abstract: In collaboration under Germanium-based Science and Technology Advancement Research (Ge-STAR) one of the goals is to explore the use of High Purity Germanium (HPGe) Detectors for medical applications. One such application is the use of HPGe Detectors as an alternative for tumor screening using Compton Scattering to distinguish between tumor and healthy tissue in addition to pinpointing the location of a tumor inside healthy tissue. This presentation is an exploration of the magnitude of effects regarding chemical composition and density on detection rates with a HPGe Detector to understand the limitations and inform the design of a device. In order to observe the detection rates for the gamma-ray interactions in matter of Compton Scattering and Photoelectric Absorption we use GEANT4 nuclear physics simulations of our detector, source, and screening sample. Additionally, these effects are observed over a range of gamma-ray energies from 55 keV to 1460 keV on varying density and chemical compositions for healthy and tumorous tissue. This analysis helps build an understanding for what metrics a screening device needs to meet its goals to improve current X-ray diagnostics with new gamma-ray HPGe detectors.

Oral Presentation
Undergraduate Student

Presentation Number: 204
Presentation Title: Developing an Accurate Microphysiological System for Studying Vasculature

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Abstract: Animal clinical trials are a crucial element of the modern pharmaceutical industry, but recent initiatives have cast doubt on their accuracy and relevance to human patients. These studies are extremely expensive and often result in the drug failing to move on to a human trial. Additionally, these early animal studies can fail to catch adverse side effects, which in turn can put human subjects at risk. For these reasons, the medical industry has been pushing for less reliance on animal models and more accurate and cost-effective testing methodologies. Microphysiological systems (MPSs) are one such device that can fit this need. MPSs are in vitro models that seek to accurately mimic a targeted human tissue or organ.
While MPSs are currently being developed as a supplement to animal testing, many such devices have yet to comprehensively account for chemical and physical forces innate to native tissue, which have been shown to impact the behavior of cultured cells. As such, research is needed to develop MPS systems that strive to accurately mimic the forces at play within the body.
These forces come into special consideration when developing MPSs to model human blood vessels. By utilizing microfluidics, these devices can mimic human vasculature. Lithography is traditionally used to carve out channels in a PDMS mold. PDMS lithography severely limits the channel layouts, resulting in flat, rectangular channels. This subjects the cells and the fluid in the channels to different mechanical signals than the cells in cylindrical, human blood vessels. In response to this, this research group has been developing a model that addresses these design flaws.
Our design process has resulted in development of MPSs with physiologically relevant length scales and cylindrical channels. However, these designs still require further improvement. Further work is currently underway to improve the usability, sterility, and data collection from these devices.

Oral Presentation
Undergraduate Student

Presentation Number: 205
Presentation Title: Dust Deposition on Radiopure Titanium

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Abstract: Minimizing radium contamination is essential for experiments such as the LUX-ZEPLIN (LZ) dark matter detector at the Sanford Underground Research Facility. Although LZ uses the purest titanium ever made, radium impurities in the titanium are believed to be the main source of background interactions. To determine the best way to remove radium from titanium in future experiments, we plan to measure radon emanation from titanium both before and after acid etching. Because dust particles emanate radon, sample surfaces must be cleaned to a level of less than one microgram of dust per square centimeter to ensure dust contribution is negligible when performing a radon emanation test of the titanium.
This project evaluates specialized cleaning techniques for preparing ultrapure titanium samples for low background measurements. Because dust particles fluoresce under UV light, I was able to determine how much dust was on the surface by taking magnified images lit by blacklight. Images taken of the titanium samples after initially using an ultrasonic cleaner showed that dust contamination was 21μg/c, over 20x too high. Powerwashing was performed because titanium is not soft enough to be deformed by a normal powerwasher, but most material adhering to the surface would be washed away. Though mineral deposits and other contaminants from the water being left behind were a concern, the amount of material left behind after powerwashing was found to be under 1μg/cm2. The next steps in this experiment are to perform a radon emanation run of the world's purest titanium in the Dakota Building cleanroom.

Oral Presentation
Undergraduate Student

Presentation Number: 206
Presentation Title: Optimization of Silk Extraction and Characterization of Dip-Coated Tubes for Tissue-Engineered Vascular Grafts

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Advisor: Travis Walker
Karen M. Swindler Chemical Biological Engineering Department

Abstract: Heart disease remains the leading cause of death in the United States, accounting for about one in five deaths. Vascular grafts are commonly used in coronary artery bypass grafting (CABG) to treat cardiovascular disease, but reliable options for small-diameter grafts are limited. The development of a functional small-diameter vascular graft requires specific material selection, consistent processing methods, and thorough characterization to ensure reproducible mechanical and biological function. Silk fibroin (SF) was selected as a biomaterial due to its favorable biocompatibility and mechanical properties. Because native SF must be extracted and solubilized to form regenerated silk fibroin (rSF) before fabrication, the protocol plays an important role in determining the final material properties. In this study, a modified extraction and solubilization protocol was developed to improve consistency. Dip coating was used to create silk tubes with a similar diameter to vascular grafts. The products of each processing step were characterized, and the properties of the rSF solution were related to the starting material and final tube performance. Mechanical evaluation of the dip-coated tubes, including burst pressure and compliance was conducted. This work emphasizes the importance of protocol consistency and material characterization in the development of reliable silk-based small-diameter vascular grafts.

Oral Presentation
Undergraduate Student

Presentation Number: 207
Presentation Title: Stellar Body Evolutions and Analysis of Carbon Burning in MESA

Student Name: Christopher Butsavage
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Advisor: Frank Strieder
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Abstract: Stellar nucleosynthesis is the process carried out by stars throughout the universe. A well-known method of nucleosynthesis is nuclear fusion. This fusion allows a star to resist gravitational collapse and continue to evolve while producing the elements that make up our universe. Studying this process grants a deeper understanding of the mechanisms that drive the lifecycles of star. Some stars will experience distinct stages of nucleosynthesis in which they can burn heavier elements depending on the mass and the amount of energy being produced by the current burning phase. Stars in the mass range of around 8 solar masses can reach the carbon burning phase in which the star begins using carbon as its primary fuel source. This has profound implications for the end-of-life result for the star as if the star has enough energy in can lead to a supernova explosion, releasing the material out into to space. The primary goal of the research is to determine the mass range for stable carbon burning in massive stars by measuring the effects of varying the nuclear cross-section of Carbon-12 Carbon-12 reactions. For this project, the open-source computational software known as Modules for Experiments in Stellar Astrophysics (MESA) is utilized. MESA simulates stellar evolution by taking in several adjustable parameters given by the user, such as the mass of the star, composition, and more. In MESA we can produce plots of important characteristics of the star like temperature vs density, or of particular interest to us abundance of material inside the star. The program allows us to save the results numerically and graphically at set intervals. My current task is to study the mass range of carbon burning. Doing this changes energy requirement for the star to reach higher levels of burning and by extension the requirement for the star to go supernovae. As it stands now, we have preliminary results that stand by our current estimated ranges, and we will continue to gather more data.

Oral Presentation
Undergraduate Student

Presentation Number: 208
Presentation Title: Preliminary Exploration of The Equitent Problem for Soap Films with Non-Convex Interiors

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Advisor: Dr. Neil Steinburg
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Abstract: Equitent problems (where “equitent” refers to both “equal content” and “equal extent”) are a type of geometric optimization problem that seek to find an area minimizing, m-dimensional hypersurface under two joint constraints: (1) the hypersurface encloses a given m+1-dimensional volume; and (2) it spans a given boundary in R^n, where $n \geq m+1$. The goal of this project is to find solutions to the equitent problem for hypersurfaces with non-convex interiors. Although we consider the equitent problem in any dimension, we put greater emphasis on 2 and 3 dimensional hypersurfaces, since these constitute the possible physically realizable soap-films. We consider a soap film to be physically realizable if it is possible to obtain the appropriate soap-film surface on a wire frame dipped in a soap solution. We develop a general construction for hypersurfaces beginning from regular polytopes (n-dimensional analogs to regular polygons) with circumradii greater than their edge lengths. Included in this construction are all the regular polygons with more than 6 vertices in 2 dimensions, and the dodecahedron in 3 dimensions. We limit the potential starting figures to regular polytopes with circumradii greater than their edge length, since these will always bring about non-convex interior regions through our construction. We attempt to prove that our conjectured hypersurfaces are in fact area-minimizing within their homotopy class using competitor surfaces and the method of metacalibration. We address the advantages and challenges of using the Knothe-Rosenblatt (KR) rearrangement on non-convex interior regions within the proof. This work is motivated almost entirely by earlier research findings in equitent problems from the group of researchers at BYU who originally coined the term “equitent”.

Oral Presentation
Undergraduate Student

Presentation Number: 209

Presentation Title: Fabrication of 2D van der Waals Heterostructure Devices via Dry Transfer Method

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Abstract: Two-dimensional (2D) materials have emerged as a versatile platform for next-generation electronic devices due to their atomically thin nature and the ability to form van der Waals interfaces without lattice-matching constraints. In this work, we assembled a 2Dheterostructure and investigated its rectifying behavior. Individual flakes were obtained via mechanical exfoliation and identified by optical microscopy before assembly. We used a pre-defined gold electrode for the fabrication of the device. The heterostructure was constructed using a polymer-assisted dry transfer method, which minimizes contamination and interlayer damage. Electrical transport was characterized using current-voltage (I-V) measurements, which reveal clear diode-like rectification. Overall, we demonstrated a 2D heterostructure device with clear rectifying behavior, showing the potential of van der Waals junctions for electronic applications.

Oral Presentation
Undergraduate Student