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2ND ANNUAL GWEN SYMPOSIUM

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Abstract Booklet

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2nd Annual GWEN Symposium: Sharing Your Voice, Extending Your Reach

Characterization of composite hydrogel-Portland cement hydration products

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Hydrogel-based internal curing agents can be used in Portland cement systems to produce microstructural refinement of the cement matrix, leading to more durable cement with longer service life. Crosslinked polyacrylamide-based hydrogel particles serve as reservoirs of water to promote the cement hydration reaction responsible for hardening and strength development. Cementitious systems are highly basic (pH ~13) with many ionic species in solution, including K+, Na+, Ca2+, H2SiO42- (ionic strength ~0.3 molal). Variation of crosslinking density and of co-polymer ionic fraction have been shown to affect hydrogel properties in cementitious systems with respect to both absorption behavior and hydration product formation within the void left in the cement matrix as the hydrogel desorbs. Using methods inspired by biomineralization research, this study explores nucleation and growth of calcium hydroxide and other cement hydration products within polyacrylamide hydrogels with the goal of improving understanding of the role of hydrogel properties in mediating cement hydration product formation. Cross-linking densities and co-polymers were varied to control localized degree of supersaturation and ion-polymer interactions. Optical microscopy and image analysis were used to quantify crystallization kinetics within bulk hydrogels immersed in supersaturated solutions including calcium hydroxide solution and simulated cement pore solution. Hydrogels and crystals were further characterized using small angle x-ray scattering and x-ray diffraction to determine the hydrogel's influence on crystal morphology as well as crystallization's influence on hydrogel morphology. Extracted crystals and dried crystal-containing hydrogels were characterized with scanning electron microscopy for morphology and thermogravimetric analysis. Results from these experiments will be presented along with implications for informed selection or design of hydrogels for internal curing applications.

An Analysis of Chemical Engineering Students' Self-Regulatory Beliefs and Processes in an Introductory Materials and Energy Balances Class

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This presentation summarizes an ongoing research project investigating students' self-reported self-regulatory processes in a materials and energy balances course. In this course, students learn how to integrate multiple complex concepts to solve chemical engineering problems. Students' ability to achieve their desired outcomes is a combination of multiple factors including content mastery, time management, and resource management. Students' learning experiences and performance in this class significantly determine their ability and intention to persist in the chemical engineering program at this university and in other chemical engineering programs nationally. Additionally, following this course, many students leave chemical engineering, especially systematically marginalized students (i.e., women, non-binary students, Black, Latino/a/x, and Indigenous students) who face additional barriers when navigating engineering disciples. This course serves as an important gateway in the chemical engineering degree progression, and as such, identifying the regulatory beliefs and processes that students employ to successfully navigate this course can provide specific ways to better support students' learning within the course.

Self-regulated learning is an internal process where learners direct their performance towards their learning goals. Self-regulated learners observe, assess, and positively respond to their learning goals in the context of their emotions, behavior, and learning environment. Prior research describes self-regulated learners' ability to focus on relevant learning tasks, seek help, and persist when facing challenging learning goals.

In this study, we examine the regulatory beliefs and processes of second-year chemical engineering students in an introductory materials and energy balances course. Data were collected across three semesters (Fall 2021 - Fall 2022) using the MSLQ (motivated strategies for learning questionnaire) and the MAI (metacognitive awareness inventory) administered at two time point during each semester. We answer the following research questions: (1) What is the relationship between students' regulatory process and beliefs in the materials and energy balances course? (2) To what extent do students' regulatory process and beliefs predict their final course grades in the materials and energy balances course?

Introducing Fundamental Quantum concepts to K-12 Students and Teachers

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Responding to the recent call of the National Quantum Initiative Act (2018) to accelerate quantum research and development, we aimed to bridge the gap between developing quantum technologies and teachers and their student's interest and knowledge in quantum-infused Science, Technology, Engineering, and Mathematics (STEM) learning contents. Towards this end, we evaluated changes in teachers' perceptions and interest in quantum-infused science learning and teaching. Using the Interconnected Model of Professional Growth [IMPG] (Clarke & Hollingsworth, 2002), we investigate the relationship between the four domains of IMPG based on teachers' new knowledge, beliefs, attitudes (personal domain), and experiences (external domain) about quantum-infused resources (i.e., summer workshop, the developed curriculum unit), their perceptions and implementation of quantum-infused learning contents (domain of practice), and outcomes after teacher implementation (domain of consequence). The authors of this paper operationalized the IMPG model in the context of the quantum-infused middle school science education initiative of Innovation in Quantum Pedagogy, Application, and its Relation to Culture (IQ-PARC) through qualitative analysis of teacher interview data. The interview data was collected after the Teachers' Quantum Workshop organized in the Summer of 2022. However, this paper specifically focused on the interactions between the personal and external domains, which refers to in-service teachers' knowledge, beliefs, and attitudes about quantum-infused middle school-level science education and their own experiences about the workshop, respectively. Data related to practice and consequence will be included in research findings later once teachers implement quantum-infused middle school-level integrated STEM units in their classrooms. Based on our qualitative analysis, we suggest future implications of teacher perspectives on quantum and quantum-infused teaching practices for developing integrated STEM education for young learners.

Optimal digital design of flexible modular mini-plants for distributed drug manufacturing

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Most of the drug products involve at least one crystallization step for purification purposes. Some of the main critical quality attributes (CQAs) for crystals are purity, polymorphic form, crystal size, crystal shape, and the distribution of size and shape. These CQAs affect the manufacturing processes and the properties of the drug products such as bioavailability, dissolution, stability, and shelf life. Pharmaceutical manufacturing typically uses batch processes and centralized facilities however, there have been recent efforts to shift manufacturing toward distributed, continuous, and smaller-volume manufacturing to address issues related to the production, supply chain, distribution, and personalization of medicines (Nagy et al., 2021). Mathematical modeling of the unit operations for mini-plants (micro-scale reactors, separators, crystallizers, filters, and dryers) is very important to reduce experimental efforts, lower manufacturing costs, and have reliable quality (Diab et al., 2019). This work aims to use a digital-twin approach for the design of modular mini-plants for distributed drug manufacturing.

The optimal mini-plant layout, design (such as unit volumes), and operation parameters are obtained by solving the optimization problem that minimizes the variance of an applicable profit index regarding the constraints (limiting the waste and the risk of producing out-of-specification drug products). Techno-economic analysis of different process design configurations is required to show the most economically viable option for the distributed manufacturing platform (Diab and Gerogiorgis, 2017). Of special interest is considering the desired flexibility of the production scale, and evaluating batch, continuous and hybrid operating modes with the scope to design end-to-end-optimal (E2EO) manufacturing systems.

A case study on a chemotherapeutic agent is demonstrated to show the potential of this digital design strategy. A python-based modeling platform, PharmaPy (Casas-Orozco et al., 2021) is used for parameter estimation. End-to-end batch, continuous and hybrid operating modes can be explored for drug manufacturing using the capabilities of PharmaPy. The optimized process is implemented in a mini-plant and process analytical technology (PAT) tools are utilized for process monitoring during model validation experiments to obtain better control over drug product quality.

Multiphase modeling of particle/air counter flow in a parallel plate fluidized bed heat exchanger

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A high temperature particle solar receiver is being developed by using a light trapping planar cavity configuration. As particles fall through the cavity, the concentrated solar radiation warms the boundaries of the receiver and in turn heats the particles. Particles flow through the system, forming a packed bed at the lower end, and leave the system from the bottom at a constant flow rate. Air is introduced to the system as the fluidizing medium to improve heat transfer and mixing in the particles. A laboratory scale cavity receiver is built and a near IR quartz lamp is used to provide flux to the vertical wall of the heat exchanger. This system is then modeled using NETL's open-source code, MFiX, using a continuum two-fluid model. The model matches the system size and assumes monodisperse particle size distribution equal to the Sauter mean diameter of the tested particles. A conduction model (Morris, Pannala, Ma, & Hrenya, 2015) that accounts for the effects of solid concentration is implemented and the heat flux boundary condition matches the experimental setup. The radiative flux contribution (John C. Chen, 2005) is included in the post processing step to calculate the heat transfer coefficient. The model is validated against testing data and achieves less than 30% discrepancy in the heat transfer coefficient values. The aim of the study is to improve the heat transfer to the particles and to this effect, very small particles like Silica (150 μm diameter) and Olivine sand (90 μm diameter) are tested. It is observed that the heat transfer to the particles is greatly dependent on the thermal contact between the particles and the heated wall, and hence the concentration of particles near the heated wall. The simulations show that the gas velocity is higher near the heated wall due to changing air properties with temperature, and this results in the formation of a weak channel, thereby reducing the solid concentration near the wall. To overcome this channeling, the system is inclined by a small degree towards the heated wall so that gravity assists in maintaining good thermal contact. This inclination is observed to significantly enhance heat transfer. Fluidizing the domain helps with particle mixing and hence also increases heat transfer to the particles and the presence of an optimal fluidization regime is observed. Particle and air flow rates, as well as inclination angle, need optimization to maximize heat transfer. The model achieves high heat transfer coefficients of more than 1000 W/m2K.

Cortical Bone Microdamage and Modulation by Hydration Thereof

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Investigating the deformation and failure of cortical bone tissue under biochemically altered hydration looks at new approaches to risk reduction in the skeletal system. Characterization of water in cortical bone can modulate biomechanical behavior and help understand how bone can dynamically change due to age, disease, and treatment. This study aims to observe hydrated ex-vivo relative to the in-vivo state: increase it by use of a compound (Raloxifene) common to osteoporosis treatment regimens; decrease it by thermal dehydration to mimic the natural loss hydration with aging. The behavior of human cortical bone under this modulated hydration state by bending mechanical loading protocols (ex-situ and in-situ for 3D observations) is used to analyze the development of strain and its complex interaction with bone microstructure, microdamage, and fracture in progressive bending tests through a loading-unloading scheme. In conjunction with mechanical testing, acoustic emission (AE) signals are acquired. The combination of AE energy per cycle places mechanical damage measurement into the context of AE measurements, and provides an immediate indication relating to the strength or risk of failure of a component. Additionally, the cortical bone bending samples is analyzed through UTE-MRI, investigating 3D spatial information of the total, bound, and free water within cortical bone samples. Using dual-echo 3D UTE acquisition, the porosity index in the bone tissue is derived and the long T2-saturated UTE is used to determine the amounts of bound and free water in the bone microstructure. This research seeks to combine methods in bone biology and mechanics of materials to solve problems of bone fragility. The integration of 3D spatial image information of water in bone with that of deformation and damage leads to new insights on how bone composition and microstructure jointly affect bone failure. New insights will be obtained into how different levels of bone hydration affect the overall permanent strains associated with damage accumulation in relation to the number of load cycles and applied level of bending. This data correlates the aggregated hydration state in bone and the spatial distribution of local strains and damage in correlation to the local hydration state in bone.

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Crop residue estimation using SAR

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Crop reside estimation is crucial as it can serve as a surrogate variable to determine tillage practices in the field. We want to propose to develop a data-driven crop residue estimation model using SAR data. We established crop residue testbeds in the mid-west region. We will collect traditional crop residue estimates using a line transect method, and we will also collect ultra-fine spatial resolution UAS data over the testbeds. This study aims to evaluate the feasibility of the ultra-fine spatial resolution UAS data to estimate crop residue by comparing field measured crop residue estimates with the UAS based crop residue estimates. If the UAS based crop residue estimates are proved to be as reliable as the manual field-measured crop residue estimates, the UAS derived crop residue estimates can generate a large number of training samples to train SAR data for developing a large scale estimation model. We believe these results will provide a valuable case study for the crop residue application of the NISAR project.

High Throughput Platform for Understanding Macromolecular Interactions with Collagen and Hyaluronan

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The emergence of biopharmaceuticals resulted in a need for advancement in administration routes of the molecules. Subcutaneous administration, while advantageous, poses challenges concerning bioavailability of the molecules due to the complex transport process. The transport of the injected therapeutic is dictated by physiochemical properties of the molecules such as hydrodynamic radius, net charge and hydrophobic characteristics. The extracellular matrix (ECM) of the subcutis is largely composed of collagen, a fibrous protein, and hyaluronan (HA), an anionic polysaccharide. The high viscosity of HA is believed to act as a barrier for therapeutic transport. Currently, in vitro, high-throughput platforms that allow transport screening through ECM models are limited.

Transwell macromolecular recovery assay is a promising method that allows for systematic evaluation of the contribution of various ECM components on the transport of macromolecules. Here, we utilize the Transwell assay with collagen, HA and combined collagen-hyaluronic acid (ColHA) hydrogels as in vitro tissue models to determine mass transport properties of label-free macromolecules. Panel of six macromolecules of various zeta potentials and hydrodynamic radii were tested. Percent recovery of all molecules was measured at five time points. Recovery rates, defined as the slopes of percent recovery data, were calculated.

In this work, we demonstrate that the transport within collagen hydrogels is governed by steric interactions, with the macromolecular recovery being inversely related to the hydrodynamic radius of the macromolecules tested. Molecular recovery through HA solution is a function of both molecular charge and size. Negatively-charged macromolecules such as myoglobin had an increased recovery compared to lysozyme, a positively charged enzyme of similar hydrodynamic radius, which likely experiences attractive forces to the negatively charged HA. Size effects persist, as negatively charged bovine serum albumin recovery was lower compared to the less negative but smaller myoglobin.

To assess the contributions of both collagen and HA simultaneously, hydrogels composed of collagen and HA (ColHA) were tested. Increasing HA content from 0 to 8 mg/mL within the collagen gels preserves the trends observed in collagen-only hydrogels but decreases mass recovery of the macromolecules. This decrease in mass recovery is mainly the result of increased viscosity. Limited charge effects have been observed at high HA concentrations within the ColHA hydrogels. Thus, the Transwell platform can be utilized to screen molecular interactions and transport properties within tissue models.

Adhesion of Recycled Carbon Fiber Reinforced Composites to Aluminum

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Carbon fiber reinforced polymer composite (CFRP) materials have found application in industries including aerospace and automotive due to their high strength and low density, replacing heavy, traditionally metallic, components with this equally high performing material. Easily processable with multiple forming options, CFRPs can be used in locations where complex geometries are required, such as battery boxes for electric vehicles. As part of forming these geometries, excess scrap material is cut off from the final part and discarded. Scrap material combined with end of service life material from thousands of planes manufactured at the onset of CFRP manufacturing will produce thousands of pounds of CFRP destined for landfills. As energy intensive materials, there is motivation to recycle these materials for secondary use likely in non-structural applications. This work aims to bond recycled CFRP materials to aluminum without the use of adhesives for light weighting in an automotive application. Avoiding the use of adhesives allows for faster and cheaper manufacturing, as well as easier recycling post service life. Current challenges to recycling CFRPs include maintaining the length of the fibers and decreasing surface defects, meanwhile challenges of adhesion of these dissimilar materials include poor wettability and mitigating differences in coefficients of thermal expansion. Literature has demonstrated the ability to overcome these difficulties proving the feasibility of both recycling carbon fiber in addition to adhering CFRP to metal substrates. The interplay between these two issues is less studied, and is therefore where this work will focus. This research is still in the preliminary phase and as such no results will be discussed, however a current plan for testing will be presented.

Hydrogel porostiy and mechanical property tuning for cell infiltration and osteointegration

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Every year 1.5 million patients worldwide receive oral and maxillofacial reconstruction for intra- and extraoral critically sized bone defects. These defects can occur due to diseases such as osteosarcoma causing maxillofacial maligancies, injuries from high speed impact or projectile blasts, or even congenital conditions such as cleft palate. Currently, a defect is surgically repaired using either xeno- or autograph bone particulate to fill the cavity, which is then encased in a titanium mesh and screwed in place with titanium screws. This approach is limited by the variability in shape, extent of surgery, and degree of bone particlulate particulate packing. Although the bone particulate signals cells to differentiate along the osteogenic lineage, tight packing of the bone particulate often leads to diminished bone healing because of poor blood vessel formation. To address the fallbacks, we developed a patient specific, osteoinductive 3D printable construct, with a cover core design. The cover and core construct was engineered to be mechanically strong to endure mastication, while also being porous to allow for cell infiltration. The core consists of a hydrogel-tricalcium phosphate composite.

This study aimed to optimize the hydrogel-tricalcium phosphate composite for improved cell infiltration and differentiation while withstanding hydrolytic degradation during osteogenesis. We hypothesized that the combination of Methacrylated Alginate (AlgMa) and Methacrylated Gelatin (GelMa) would provide a robust hydrogel to support cell infiltration and that FGF containing PLGA microspheres could be used to develop a GF gradient to induce chemotaxis into the construct.

The GelMa was synthesized by combining gelatin (SigmaAldrich, Massachusettes, USA) and methacrylic anhydride and then dialyzed for a week to remove unreacted Ma. Finally, the GelMa was lyophilized for storage and future use. The AlMa Medium Viscosity 20-40% methcrylation was purchased from SigmaAldrich (Massachusetts, USA). We used an AR-G2 TA instruments Rheometer to acquire the elastic and storage modulus of AlgMa/GelMa blends. The disks were placed in 1 mL of 1X PBS buffer and at 1, 2 ,4, 6, 8 hours and 1, 3, 7, 10, 14, 17 and 21 days, the entire sample volume was sampled and then replaced with fresh buffer to maintain sink conditions. We tested the pH, sample swelling and degradation. Additionally, fluorescent recovery after photobleaching (FRAP) was performed with FITC-dextrans of different molecular weights (10 kDa, 40 kDa and 150kDa) to measure the diffusivity of the hydrogels using a Zeiss Confocal LSM 880 (Jena, Germany). Cell migration experiments were performed using Ibidi chemotaxis slides (Gräfelfing, Germany) using GFP expressing NIH 3T3 murine fibroblasts.

We observed that by manipulating the AlgMa/GelMa ratio that the porosity of the gel could be tuned to improve FGF-2 release and facilitate cell infiltration. These findings suggest through the use of this composite, early cell infiltration can be increased and promoted due to FGF release, leading to increased osteointegration.

Cislunar Space Surveillance

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The increasing number of launches around the Moon has generated a need to surveil the cislunar space for active utilization of space. Cislunar space is the region of space between the Earth and the Moon, including the vicinity of the Earth and the Moon itself. It expands to 9 times more linear distance than a Geostationary Earth Orbit (GEO) and is 1,728 times larger than the volume of space within 1 GEO. The dynamics in the cislunar space is not simply guided by perturbed two-body motion, which in turn, gives rise to trajectories that are not Keplerian in nature. The gravity of the Moon, the Sun, the Jupiter, and solar radiation pressure start having a significant effect on the orbits. Due to multi-body dynamics, trajectories in this region are not stable either. Additionally, a single sensor cannot observe all the cislunar space. Therefore, tracking and detection techniques from the Near-Earth region cannot be directly applied to the cislunar space objects.

This paper is based on previous papers which investigate conditions for successful Space Domain Awareness by employing the brute force method on visibility. This means checking visibility conditions for each location in space from all the sensor locations at each epoch which is computationally expensive. A high fidelity-dynamic model (which uses the gravity of Earth, Moon, Sun, Jupiter, and solar radiation pressure) is used with a global network of sensors. For visibility, besides the overall magnitude, the background irradiation from the sky due to the moonlight along with the limiting telescope magnitude and the nighttime constraint for objects above the horizon are also incorporated. The detection limit is directly dependent on the Signal-to-Noise Ratio (SNR) and is dictated by the exact setup of the optic's aperture, sensor type, and sensitivity in combination with the specific image processing software.

In this paper, the geometry of the Bi-Circular Restricted Four Body Problem (BCR4BP) is used to parametrize the visibility conditions and cislunar space to reduce the cost of computation. BCR4BP models the gravitational effects from the Earth, the Moon, and the Sun simultaneously. These three bodies directly affect the illumination conditions on a spacecraft/debris. BCR4BP is a higher fidelity model as compared to the circular restricted three-body problem. It is also time-dependent which is required for taking observations based on the location of Earth-Moon-Sun. A general formulation of the problem is derived to generate a map of visible locations in cislunar space given the geometry and reflective properties of an object. These maps help in finding regions of more visibility than others in the cislunar space.

Human Factors Research at the Mars Desert Research Station

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As humans continue to push farther out into space with the goal of reaching Mars, a critical step is understanding how space travel affects human health and performance. Stressors such as high workload, circadian misalignment, interpersonal team dynamics, confinement, isolation, and extreme environments can threaten the ability of astronauts to sustain high levels of cognitive performance and physical durability over prolonged periods of time. It is essential to explore human adaptation to extreme conditions in relevant environments on or near to Earth before undertaking extensive Mars exploration missions. Over the course of two weeks in January 2023, seven Purdue University researchers will conduct a series of experiments in the confines of the Mars Desert Research Station (MDRS), a space analog facility in the Utah desert, owned and operated by the Mars Society. Situated in a locale that serves as an actual analog of the Martian geological environment, MDRS enables the practical study of some behavioral and physical side effects of space travel in a realistic setting, including the challenges associated with long-duration missions. In this study, researchers will carry out human factors studies throughout the MDRS Crew 272 two-week mission, including daily administration of a computerized neurobehavioral test battery to measure vigilance, spatial orientation, and mental workload; self-reporting of perceived workload and performance; physiological assessments based on continuous smart tracker data; and response to unanticipated simulated stressors. The results of such a study could provide crucial data about the strength and validity of proposed manned missions and can inform changes in the way missions are scheduled and organized, the way astronaut teams are formed, the way habitats are arranged, and the way astronaut physical and psychological health and function are evaluated and supported during long duration spaceflight.

First-Principles Analysis of the Ammonia Decomposition Reaction on High Entropy Alloy Catalysts

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The development of periodic Density Functional Theory (DFT) calculations, combined with advanced synthesis techniques, has accelerated the understanding and development of multimetallic alloy catalysts. Recently, a new class of materials, known as high entropy alloys (HEAs), has opened up additional catalyst design possibilities in the alloy space. HEAs are comprised of many principal elements, with completely mixed atomic structures, leading to potentially millions of unique chemical environments around active sites. These materials have attractive properties for catalysis, including enhanced stability due to entropic effects, as well as highly tunable active site structures that could be exploited to optimize catalytic activity and selectivity. Nevertheless, the huge materials space cannot be navigated exhaustively using first-principles methods, and the scaling theories and models proposed for traditional alloys may not be directly translatable to HEAs.

In this study, we systematically develop a model of high entropy alloy catalysts, and randomly-ordered bimetallic alloys, and subsequently extend these ideas to incorporate multiple elements. Additionally, we develop tools to efficiently sample different binding sites and investigate the free energy landscape for simple adsorbates on these sampled sites. To illustrate this approach, we choose the ammonia decomposition reaction as a probe reaction and Co-Mo as a model catalyst, based on the promising activity demonstrated experimentally for this chemistry on Co-Mo-based HEAs. We determine the binding energies of various reaction intermediates on many randomly sampled arrangements of the HEA surfaces using DFT. We deduce that the rate-determining step for the ammonia decomposition reaction is recombinative nitrogen desorption. This conclusion remains constant across the different considered surface arrangements. The results form a strong basis for further studies and the development of high entropy alloy catalysts for ammonia decomposition.

Utilizing Transdisciplinary Project-Based Learning in Undergraduate Engineering Education

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Transdisciplinary project-based learning is an opportunity for undergraduate engineering students to acquire valuable skills in translating individual knowledge to other disciplines and interacting with non-academic stakeholders. In the authors' project-based education experience, these skills have been developed in both course-based and co-curricular learning contexts. Drawing from published studies and course frameworks, as well as the authors' student experiential perspectives, understanding what effective transdisciplinary project-based complementary experiences are and how they shape engineering undergraduate students as cross-disciplinary, holistic problem-solvers are the primary emphases of this paper. The necessary foundation to implement transdisciplinary projects in education is introducing students to collaboration across disciplines as well as with stakeholders, consumers, and users. Furthermore, students are supported through the learning of holistic problem-solving techniques by their team and professors through scaffolding teaching methods. Emergent behaviors are inherent to complex real-world problems. Engineering students would benefit from the opportunity to practice adapting to evolving project requirements and goals in low-risk, academic settings prior to enduring these challenges at the career level. This active learning approach can increase student agency and diversity as students work in multi-disciplinary teams on relevant problems with social, environmental, economic, or political implications. Relevant problems encourage students to draw from previous experiences and knowledge during problem and user discovery. Additionally, students learn the value of qualitative data in these investigations for characterizing exigencies of stakeholders, consumers, and users that are often unavailable from quantitative data, though generally more emphasized for use in engineering design decisions. Students participating in transdisciplinary project-based learning gain insight, agency, and develop a skill-set for investigating the cross disciplinary implications and socio-technical contexts of real world problems.

Controlling Quantum Emitter Performance In Nanophotonic Cavities For On-Chip Cavity QED

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Strong coupling between solid-state quantum emitters and nanophotonic cavities paves the path for coherent manipulation of quantum state for on-chip photonic quantum information processing. Performance of such bosonic systems depends on Purcell Enhancement, Cooperativity factor and operating regime for production of reliable quantum emission in the form of single photon, bi-photon or controllable multi-photon states. Such quantum state production is essential for quantum communication and optical quantum computing circuitry   with tunable polarization, shape, and coherence time. One of the core issues of on-chip photonic quantum information processing is reliable and deterministic control of emission rate and lifetime modification of quantum emitters. Over the last decade, modulation of local density of states in a nanocavity has been explored and modelled theoretically for this purpose, using Wigner-Weisskopf approximation. Previous experiments have shown spontaneous emission of cavity-coupled Quantum dots have been enhanced around 8 times compared to quantum dots in bulk GaAs. This coupling between a quantum emitter and a cavity open path for more fine-tuned single photon sources as well as reliable entangled photon pair generations with higher out-coupling efficiency between the coupled cavity-emitter system and the waveguide apart from increased visibility of spectrum. On the other hand, decoupled quantum dots emit upto five-fold decreased rate compared to bulk quantum dots.

Here we present a numerical study comparing semiclassical and quantum models of a damped cavity strongly interacting with a quantum dot and operating at telecom wavelength for further application in complex quantum networks as well as quantum bio-imaging for NIR-II region. Our cavity consists of a silicon photonic crystal nanobeam with 1D photonic bandgap extending from 1200 nm - 1700 nm following experimental data. Considering recent breakthrough in tuning quantum dot emission at that regime, we proceed toward modelling our proposed Cavity-QED system with FDTD based numerical method for extracting parameters such as coupling between atom-cavity system, condition for weak, strong and ultra-strong-coupling in the system, mode volume, full-width half-max cavity energy decay rate, Quantum Emitter's efficiency and effect of phononic perturbations on optimizing photon generation efficiency and possible quantum gate implementation while enhancing performance of the system. A major goal of our cavity design was to enhance quantity factor over a million while trading on mode volume as minimum as possible to maximize cooperativity. However, we further consider maximizing photon generation efficiency in the system while trading off co-operative factor to achieve optimal decay of the quantum emitter from the cavity towards an unprobed waveguide that may further process the emitted photons for applications in quantum circuits.

We use Meep to design the cavity structure to maximize the quality factor (Q) of the fundamental resonant mode. We further modify and play with the geometry to control and manipulate the photonic bandgap as well as resonance frequencies in order to accommodate the recent development in quantum dot emission engineering for visible to the second NIR optical window region.We are optimistic about application of our proposal for on-chip quantum information processing.

Inclusivity and accessibility of Virtual Reality

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Virtual Reality (VR) is fast becoming a household name in the world of technology. For example in entertainment, games like Beat Saber, Pistol Whip, etc. have been shown to have positive impacts on the lives of people. In a report on the proceedings of the 5th International Conference on Multimedia, the research studies show that VR not only promotes mental health and improves anxiety but is also relatively safe and there are few negative effects from using the technology.

The future of VR is very promising and with VR being more incorporated into the various aspects of human life, it is only a matter of time before VR becomes conventionally integrated into the everyday life of humankind. Therefore, it is imperative for Human-Computer Interaction (HCI) researchers to understand how VR can accommodate more accessible and inclusive designs for a diverse users. This presentation dives into the utilization of VR for minority groups in the old age population. It also touches on some ways VR games can be more adaptive to wheelchair users with upper limb impairments.

The overall impact of this work is to direct the attention and focus on populations that are under-represented in the realm of Extended Reality (XR: Augmented Reality/ Augmented Reality/ Mixed Reality (MR/VR/AR)). The research philosophy in this project is centered on applying empathy to accessible and inclusive design.

The research studies discussed in this presentation aim to highlight the power of compassion when bringing value to underserved users. Another gap that this presentation aims to fill is to invite the perspectives of users typically excluded in technology design to inform an equitable design and research process in the domain of XR.

Analysis of Contaminants on Ground Glass Pozzolan and the Effects on Pozzolan Performance in Mortar

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Using ground glass pozzolan as a replacement for portland cement can reduce the CO2 emissions associated with concrete production and utilize waste glass that would otherwise end up in landfills. In the United States, municipal solid waste (MSW) stream recycling operations collect plastic, glass, paper, and other recyclables together in single stream recycling. Glass collected in this manner can contain an unknown concentration of various contaminants on its surface, which can cause concern for concrete producers concerned about the effect on performance. Using analytical chemistry techniques combined with mortar physical testing, it is possible to better understand what kinds of contaminants are present on recycled glass and how they affect cement mortar compressive strength. Primary targets of contaminant analysis were surfactants and carbohydrates such as sugars and cellulose. Gas chromatography-mass spectrometry (GC-MS) was used to assess the presence of the surfactant sodium dodecyl sulfate and glucose. Colorimetric phenol-sulfuric acid assays (PSA) were used to detect and quantify the amount of carbohydrates on the surfaces of the glass pozzolans. Results indicate carbohydrates to be the primary contaminant on the recycled glass surface, with glucose being a confirmed contaminant using GC-MS. Using the contaminant concentrations determined through analytical techniques, contaminant-dosed mortars were produced, and the effects on compressive strength and flow were measured. It was found that samples dosed with 0.5 wt.% glucose had decreased compressive strength at day one but gained strength over time and reached or surpassed compressive strengths similar to control mixes by 28 days.

Crack Growth in Human cortical Bone: In-Situ Loading with 3D imaging

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Treatment of osteoporosis commonly focuses on increasing bone mass, but assessment and improvement of bone quality is also key to effective outcomes. Several mechanisms are known to contribute to bone toughness, a key property for assessing fracture risk, but evaluation of these mechanisms across length scales can be hindered by the limitations of imaging. In the present study crack growth resistance is measured in human cortical bone with specimens of relavent physiological size. Fracture initiation and propagation is evaluated with in-situ 4 point bending and concurrent 3D X-ray microscopy.

Human cortical bone toughness was evaluated through in-situ laoding with 3D X-ray imaging. A human cadaveric femur was obtained through the Indiana University School of Medicine Body Donation Program from a 92-year-old male. The femur was sectioned into 4 x 4 x 28 mm3 beams, and then notched to half the height for fracture tests according to ASTM standard. Imaging was conducted using a 3D X-ray microscopy system fitted with an in-situ loading rig in a 4 point bending configuration. Beams were loaded stepwise until failure; between each step, 3D Xray imaging was performed. Image processing and segmentation was performed to distinguish microstructure and crack development throughout the loading protocol. Effective and maximum crack length, and crack mouth opening displacement were measured. Elastic modulus and crack growth resistance curves were then calculated.

All specimens exhibited a rising R-curve (increasing toughness). The 3D reconstruction of the cracks formed in the cortical bone revealed a complex 3D crack structure. These images indicate that crack initiation is determined by local microstructure. In contrast, the crack growth resistance behavior is determined by whole bone microstructure and several toughening mechanisms occur concurrently during fracture. The mechanism interactions lead to large scale crack bridges formed when entire osteons (tubular structured building blocks of bone) are locally debonded but remain intact in transmitting loads across the crack faces. These large-scale bridging events exert a shielding effect and the rising R-curve is attributed to the presence of such features.

We find large scale crack bridging events have a major impact on the fracturing of cortical human bone. Such information cannot be gained from 2D or post-fracture 3D scans. Consequently, bone microstructure has a strong influence on fracture with crack deflection at cement lines being a main mechanism. Any bone treatment should seek to preserve, or enhance, the presence of this toughening mechanism. The present study demonstrates that evaluation of bone fracture requires specimen dimensions on physiologically relevant scales and the need for 3D imaging of cracks. Only then can relevant mechanisms and their effects on bone quality be assessed across length scales. Improving bone toughness - and therefore resistance to fracture - is critical to addressing bone related disease. As the predictions of fracture incidence rise, addressing bone toughness improvements will benefit those with bone diseases such as osteoporosis.

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A computational framework of electrochemistry and mechanical degradation in Li ion battery NMC cathodes

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Li-ion batteries are the most successfully commercialized rechargeable batteries, especially in the market of portable electronics and electric vehicles. Researchers of batteries are motivated by the imperative demands of high energy density, fast charging, long circle life, and low cost. LiNixMnyCozO2(NMC) is an outstanding candidate for cathode materials of Li-ion batteries due to its high energy density, favorable operating cell voltage, low cost, and tunable properties. The capacity decreases of NMC cathodes mainly origin from mechanical degradations, such as intergranular fractures. During charging process, extraction of Li from NMC cathode particles would induce the lattice deformation, which is considered as delithiation strain and may further induce mechanical stresses. The intergranular fractures are mainly induced by the mismatch strains between the randomly orientated primary particles. The intergranular fractures slow down and even cut down the pathway of Li, which increase the polarization and reduces the available capacity of batteries. Furthermore, serious fractures will isolate the primary particles from surrounding particles and the capacity of this isolated particles gets totally lost, which is a huge damage to the battery's capacity. In this work, we simulated the kinetics of Li-ion concentration transport and surface charge transfer, stress field, and intergranular fractures by using the finite element method with a coupled electro-chemo-mechanics model at the half-cell scale. In the meantime, we want to evaluate the effect of anisotropic materials properties, such as anisotropic diffusivity, anisotropic mechanical properties, and anisotropic delithiation strain, on Li kinetics, mechanics, and electrochemistry performances. From which, we find the concentration and stress profiles are very different between the anisotropic and isotropic modeling, which indicates that the anisotropic materials properties are important features to include. We also simulate the cyclic behavior of particle fractures. The fractures mainly show up in the first charge and remain stable in the following cycles.

Model-directed experiment to measure particle flow behavior

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Particulate materials are commonly used in the production of consumer goods since they are easier to transport and shape than solid materials. Predicting how a certain particulate material will flow is very difficult since the flow behavior is dependent on variables such as the size distribution, shape, surface roughness, and density of the particles.

Many commercial rheometers are on the market that can measure flow properties, but the usefulness of the data largely depends on the geometry of the device. Currently, no single rheometer can give enough information to be applicable to all applications.

Computer simulations have also been used to model particulate flows. One common model is the discrete element method (DEM) in which individual particles are modeled and collectively used to study bulk behaviors. These computational models are limited to simple particle shapes (spheres) and often make approximations about the particle properties that while make computation easier, are not fully representative of the system.

In this current work, a rheometer was designed and built to measure particle flow behavior. The device includes multiple sensors located along the boundaries of the device that can measure the bulk particle resistance to and applied shear force. During the initial design process, a DEM model was used to simulate how the proposed device would work.

In the experiments, we can capture the particle-wall interaction stress along one of the device walls using a pressure mapping sensor. Results have shown that we can identify where particle stresses are the highest and how these regions change in response to the applied shear rate, particle properties, and device geometry.

One question from the experiment is whether we can get information about the internal force network of the particle bulk using just the boundary sensors. Unlike experiments, simulations have fewer measurement limitations and can get directly analyze the internal structures. By using information from both simulation and experimental data, we hope to make the connection between the internal and boundary flow properties.

Characterizing tuberculosis granuloma dynamics using computational modeling

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Tuberculosis (TB) is the 2nd most deadly infectious disease behind Covid-19 with ~10 million new cases and ~1.5 million deaths worldwide in 2020. The host immune status is an important determinant in the formation of granulomas during M. tuberculosis (Mtb) infection. Granulomas are unique microenvironments orchestrated by the immune response to contain Mtb and localize host-pathogen interactions. Approximately 90% of individuals infected with Mtb harbor granulomas that control bacterial spread, resulting in asymptomatic disease known as latent TB infection (LTBI). In vitro studies with human primary cells infected with Mtb have shown that cells from LTBI individuals can better control Mtb growth compared to cells from naive individuals (those never exposed to Mtb before). But identifying mechanisms behind these differences is challenging.

We use an agent-based computational model of these complex in vitro granulomas to help elucidate differences between LTBI and naive host cell responses. Our computational model mimics Mtb infection through interactions between virtual macrophages, CD4+ T cells and Mtb. Mechanisms include Mtb growth, macrophage phagocytosis resulting in Mtb death or macrophage infection, macrophage and T cell activation, T cell proliferation, and cytokine/chemokine diffusion and degradation. Preliminary results showed that early activation and proliferation of TB-specific CD4+ T cells drives early activation of infected macrophages that results in more Mtb killed, larger granulomas and faster granuloma formation in LTBI-like simulations compared to naive-like simulations. Additionally, results showed that many macrophages at a low activated killing probability are better at Mtb killing than fewer macrophages at a higher activated killing probability. Parameters that may have contributed to the quick activation of TB-specific CD4+ T cells and infected macrophages in LTBI-like simulations include: lower doubling time for CD4+ T cell proliferation and lower CD4+ T cell deactivation probability. Coupling computational modeling with experimental efforts could accelerate new treatment discoveries.

Surviving the Unexpected- Designing and Implementing Safety Controls with Resilience Power

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Space habitats will face unpredictable environments while being tightly coupled and resource constrained. Therefore, it's unlikely that the habitats can be designed with many redundant safety controls, or with safety controls that address every possible hazard. Our proposed approach helps identify controls that are likely to be effective against both foreseen and unforeseen hazards. We model systems from a state-based perspective where the system is in one of four distinct types of states at a given time: nominal, hazardous, safe, or accident. Safety controls prevent the system from entering or remaining in a hazardous or accident state or transition the system to a temporary safe state or to a nominal state.

We have established an extensive database of disruptions that could affect a lunar habitat, associated safety controls, and a control effectiveness measure which evaluates the effectiveness of a safety control in addressing the hazard for which it is designed.

To address the challenge of unforeseen hazards, we are developing ways to design and select sets of safety controls that effectively address hazards for which they were not originally designed. Our hypothesis is that such high "resilience power" safety controls will result in habitats with high resilience. For an initial estimate of resilience power, we implement each safety control for multiple disruptions and record its control effectiveness for each disruption. We are studying concepts from literature on flexibility and agility to refine our measure for resilience power, and to identify ways to design safety controls with high resilience power.

Habitats with high resilience power and control effectiveness safety controls should be resilient to both foreseen and unforeseen hazards if our metrics are well-designed. We are testing this hypothesis by running simulations on RETHi's three test and simulation platforms: the MCVT, CDCM, and CPT.

Predicting Case-mix Resident Service Need in Nursing Homes

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Preparing appropriate nursing staff is vital in US nursing home management. Having sufficient nursing staff with the appropriate competencies is crucial to assure resident safety and avoid staff burnout. In this work, we present a novel approach to predict the need-based staffing time from various nursing home data resources. We first provide a conversion tool that converts the nursing home daily service census from resident individual assessment data. These data are nonstationary, count time series data with potential correlation in groups. We then provide computational insights into nonstationary service census forecasting and justify the superiority of the proposed multivariate dynamical count time series models. We demonstrate the value of our approach over Indiana's nursing homes' historical assessment and aggregated staffing data. We also obtain generalizable insights by applying the tool to a broad range of nursing home types.

Thermocouple-Based Anomaly Detection in Fused Filament Fabrication

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Fused Filament Fabrication (FFF) is a type of extrusion-based additive manufacturing process. It is often used in prototyping and other low-risk applications because of its low-cost materials, ease of use, and ability to create complex geometries. However, inconsistencies in print quality have kept this versatile method from expanding into many practical applications, as it is often unable to reliably produce high-quality parts. This research seeks to address this problem by using in-situ monitoring to identify the physics-based thermal parameters within the printer itself that lead to defects in the final printed part. Thermocouple (TC) arrays were integrated into the print bed and hotend of a Prusa iMK3S+ printer to measure temperature gradients and oscillations. The TC array in the print bed was used to identify temperature gradients (hotspots and coldspots) in order to determine their effect on the adhesion of the printed part to the print bed. It was also used to identify instances of heat accumulation, where printing multiple objects at the same bed location in rapid succession causes abnormally high bed temperatures and local melting of the print surface, despite the temperature being set to a value below its melting point. A separate TC array was integrated into the nozzle, heat block, and heat sink of the hotend to measure its temperature profile. The hotend was repeatedly heated and cooled during a print depending on the temperature set point, and the effect of the oscillation magnitude on the filament extrusion rate was investigated. In addition, the role of temperature gradients in the hotend on excessive heating, and subsequent premature filament melting, was examined. The thermal data collected from these arrays made it possible to develop a more thorough understanding of FFF by identifying parameters that could be used to create a physics-based model of the printing process. Such a model can then be used to implement closed-loop feedback control across machine designs, which will increase the probability of producing consistently manufactured, high-quality parts.

BBB-on-a-Chip: An in vitro Blood-Brain Barrier Model After Traumatic Brain Injury

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Traumatic brain injury (TBI) is a growing global health concern. TBI has been shown to increase the likelihood of the development of neurodegenerative diseases like Alzheimer's disease (AD). Moreover, the incidence of TBI has significantly increased from 1990 to 2016 globally, particularly in middle and low-middle income countries. TBI causes brain damage through both "primary injury"mechanisms, or damage resulting from mechanical insult, as well as through "secondary injury" mechanisms, or damage resulting from the release of factors after the initial mechanical insult. Both mechanisms are thought to damage the blood-brain barrier (BBB), which surrounds brain capillaries and regulates molecular transport between brain tissue and the systemic circulation. TBI models have demonstrated that the permeability of the BBB increases due to both primary and secondary injury mechanisms. Previous work in a blast injury mouse model from Uzunalli, et al. suggested that neuroinflammation resulting from secondary injury may contribute to long-term BBB damage that leads to neurodegenerative pathologies. However, limited work has been done to study the effects of secondary injury on the BBB independently from primary injury mechanisms. In this study, an in vitro "BBB-on-a-chip" platform will be developed to determine the mechanisms by which secondary injury alters BBB permeability and neuroinflammation independently of primary injury. To model secondary injury, primary neuron cultures from mouse embryos will be subject to impact injury using the TBI-on-a-chip model developed by Rogers, et al. Conditioned media (CM), or media obtained from these impacted neuron cultures four hours after injury, will be added to mouse endothelial cell and glial cell cocultures. Changes in this model BBB's permeability and protein expression will be analyzed. This novel "BBB-on-a-chip" platform will enable mechanistic study of secondary injury and will provide insight into therapeutic targets to prevent long-term neurodegeneration after TBI.

Development of Vision and Eye Care Devices in Soft Contact Lenses

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The eyes provide rich physiological and broad diagnostic information, making contact lens sensors a promising disease diagnostic tool. A smart contact lens, one such contact lens sensor, can quantify the concentrations of various biomolecules in ocular fluids and physical biomarkers of the eye, such as intraocular pressure. Continuous and non- or minimally invasive contact lens sensors can be directly utilized in a clinical or point-of-care setting. However, smart contact lenses lack practicality for patient use due to the field being relatively new and underdeveloped. Here, we introduce the incorporation of contact lens sensors and their fabrication, sensitivity, power source, and readout mechanisms. The incorporation is to monitor glaucoma and conditions associated with eye health, such as dry eye syndrome and inflammation. The resulting soft contact lens sensors fit seamlessly across different corneal curvatures and thicknesses in human eyes. The lens can also wirelessly capture the intraocular pressure by utilizing the principle of the capacitor and mechanical deformation under ambulatory conditions. Also, we will discuss the colorimetric ocular electrolyte sensors to detect the color change of dry eye disease and inflammation. We assessed the in vitro biocompatibility, ex vivo functionality, and in vivo safety of the soft contact lens sensor.

Steel Concrete Composite L-Joint Connection

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Developing effective protective structures is critical for many industries including nuclear powerplants and defense-related facilities. Steel-concrete composite (SC) elements are emerging as a viable technology for these applications. SC elements are advantageous in these scenarios because of their efficient construction schedule when compared to conventional reinforced concrete elements. Steel modules are prefabricated, shipped to the site, erected, and then filled with concrete, limiting onsite construction need as formwork and falsework are not necessary. Before applying SC elements to these structures, it is important to understand how they perform under blast and impact conditions. This presentation discusses ongoing research into SC to SC corner connections, or L-joint, for these blast and impact scenarios. Successful connections are connections that are able to undergo significant deformation prior to failure. This ductility is important in blast design because it allows for larger displacements of structural components as opposed to a sudden failure or collapse in a structure. Both experimental tests and finite element approaches will be discussed. The implication is recommendations for connection detailing and reinforcement to achieve ductility.

A test matrix has been developed with variables of interest including reinforcement details in the connection joint region, two SC wall thicknesses, numerous steel faceplate thicknesses and strengths, as well as different concrete strengths. There are three potential failure modes that are anticipated: (1) developing plastic hinges at the interface of the joint and the SC elements outside of the joint region, (2) out of plane shear failure in the SC elements outside of the joint region, (3) joint failure. The preferred failure mechanism is developing the plastic hinges in the legs. This is achieved by developing the tensile moment capacity of the specimen at the interface of the joint region of the connection. An alternate failure is joint failure. Without the presence of joint reinforcement, this failure type is characterized by concrete failure in the joint. When there is joint reinforcement, the failure mode corresponds to reinforcement yielding. Lastly, these connections could experience shear failure in the SC elements outside of the joint region. Pre-test calculations were performed for each test specimen to predict which of the three failure modes would govern. Finite element analyses were completed in ABAQUS to support these predictions and provide more insight for how experimental specimens might behave. A major finding was that a diagonal plate must be included in the joint region of specimens in order to avoid joint failure and achieve a ductile failure mode. Additionally, the reinforcement in the joint does not always prevent out of plane shear failure in the leg.

An experimental program is currently being developed to further confirm these findings. Initial testing results will be included in this presentation as well as benchmarked finite element analysis.

Deep Learning Cardiac Segmentation of Dual Ultrasound and Photoacoustic Image Data

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1. Introduction

Though methods exist to extract regions of interest (ROI) in cardiac left ventricle (LV) endo- and epicardial boundaries in ultrasound (US) images, they are still often time-consuming and cannot obtain functional information like myocardial oxygen saturation (sO2), a common focus in cardiac disease states. Photoacoustic tomography (PAT), however, can visualize sO2 in a region of tissue. Here, we highlight the capability of deep learning methods to improve LV anterior wall analysis through segmentation of preclinical murine US and PAT images.

2. Materials and Methods

The dataset used in this study consists of long-axis US and PAT images (400 each) of murine cardiac LVs acquired by a Vevo LAZR-X system (FUJIFILM, VisualSonics) and manually segmented ground truth binary masks of the anterior myocardium via a custom MATLAB script each split into training (80%) and validation sets (20%). These images and masks serve as input to a U-Net deep neural network which generates predicted masks to be used as ROIs that would otherwise have to be manually segmented. Initial testing has been achieved on a down sampled set of images (240 x 160 pixels) on a personal computer with an NVIDIA T500 using PyTorch. Following a similar approach as outlined, segmentation of reverberation artifact on a smaller set of 200 PAT images was achieved in which generated masks were applied to remove artifact. Accuracy and dice score metrics were used to evaluate algorithm performance.

3. Results

An accuracy of 98.8% and a dice score of 0.864 were achieved for myocardium segmentation while an accuracy of 98.9% and dice score 0.936 were achieved during reverberation artifact segmentation.

4. Discussion and Conclusions

Results show that training on overlayed US/PAT images using U-Net provides a model for predicting ROIs that can be used to segment the myocardium of the anterior LV wall in murine cardiac datasets and remove unwanted artifact. Limitations include a small time delay between US and PAT acquisition time. The algorithm will be run on Electrocardiogram-gated Kilohertz Visualization images to improve the time resolution of the data and algorithm performance via post- and pre-processing methods for analysis of LV wall compositional metrics like oxygenation during various cardiac disease states.

Dominant scattering mechanisms in InSbAs quantum wells

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Quantum computing has the potential to perform certain computations exponentially faster than a classical computer. The major challenge is that the building block for a quantum computer, a quantum bit, is highly sensitive to disturbances from the environment, which leads to destruction of quantum information. An approach to solving this problem is topological quantum computing. Topological systems protect information from perturbation, making them less susceptible to loss of information. In this talk, I will show why the two-dimensional electron gas (2DEG) confined in $InSb_{1-x}As_x$ quantum wells is a promising platform to achieve topological quantum computing. Desirable properties are stable device operation and low disorder. The quality of the material and the dominant scattering mechanisms will be studied in a series of quantum wells while varying the concentrations of the arsenic mole fraction with x = 0.05, 0.13 and 0.19. The electron's mobility is a key parameter for quantifying the materials' quality, and its dependence with electron density allows us to identify the dominant scattering mechanisms in the system. The data indicate that alloy disorder is the main source of short-range scattering and an alloy scattering rate of τ_{alloy} = 45 nm^{-1} per % is extracted, which estimates the alloy disorder in the system.

Solution Processed Ag2ZnSnSe4 for Scalable Solar Panel Manufacturing

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Introduction:

In 2020, 40% of new electricity generation capacity was from solar photovoltaic (PV) devices (solar panels), consisting of 28% from utility scale PV and 12% from distributed PV (e.g. rooftop, other small scale). This widespread adoption is not simply out of altruistic concerns about greenhouse gas emissions, as utility scale silicon and thin film PV are both economically viable when considering levelized cost of electricity, a measure of lifetime costs to produce a unit of energy (including installation and manufacturing). In fact, both technologies have been cheaper than coal for several years and continue to decrease in cost. Most PV devices currently on the market are based on silicon wafer technology, which requires expensive, high temperature processes, which cannot be run continuously in the manner of a printing press. In contrast, thin film photovoltaic materials have garnered much interest recently due to their processability in addition to good material properties for converting solar photons to usable energy.

Research significance:

Ag2ZnSnSe4 (AZTSe) has been made through other methods, but this presentation will discuss how we made the first stable solution of silver, zinc, and tin precursors that can be baked to produce AZTSe. Solution processing with dissolved precursors is an appealing method for future commercialized technologies due to its scalability and flexibility in methods of printing. AZTSe is additionally interesting because semiconductor devices such as solar panels require 2 types of materials (p-type and n-type) to create a junction, and other current solution processed materials are mostly p-type, requiring the n-type partner to be produced through a more expensive vacuum process. AZTSe could be a viable n-type material for existing p-type materials such as CuInGaSe2 (CIGSe).

Methodology: We solution processed AZTSe by dissolving precursors including silver, zinc, tin, and sulfur, then coated this solution on glass, and baked it at about 300C to make a crystalline Ag2ZnSnS4 material. This was annealed in an argon vacuum with additional selenium to produce AZTSe. Analysis techniques include x-ray diffraction on solids, and a number of liquid analysis techniques electrospray ionization mass spectrometry (ESI-MS), proton nuclear magnetic resonance (1H-NMR), and extended X-ray absorption fine structure (EXAFS).

Key findings: We find we are able to individually dissolve zinc metal, tin metal, and silver sulfide precursors to produce stable solutions of metal thiolate complexes. We analyzed these solutions for a deeper understanding of the individual metal complexes and interactions between them than we previously had with other materials.

Implications: The techniques used in this work can be used for other solution processed materials to better understand how to improve processing of an individual material. This work shows how interactions in each processing step between individual atoms are important in photovoltaic materials specifically.

A Brief Introduction to Multiobjective Simulation Optimization Problems

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Simulation (stochastic) Optimization (SO) problem is loosely a nonlinear optimization problem in which objective and constraint functions are expressed implicitly using a stochastic simulation model. We can refer to the stochastic simulation model as a stochastic oracle which is controllable in the sense that it has inputs that affect the functioning of the simulation model. The simulation model can be a physical experiment, Monte Carlo oracle, or any function deals with randomness. Due to the highly general formulation, the SO problem arises in a wide range of applications. Stochastic optimization is a vast topic that includes many subtopics; one of them is Multi-Objective Simulation Optimization (MOSO). The MOSO deals with the nonlinear multi-objective optimization problem in which multiple simultaneous and conflicting objective functions can only be observed with a random noise. There are different flavors of the MOSO problems based on the assumptions on the objective functions and decision variables. Based on decision variables, generally, problems are categorized as categorical, integer and, continuous problems. The Single Objective Simulation Optimization (SOSO) literature is well studied, and there are many state of art algorithms widely used in the industry and academia. However, MOSO is not well developed like SOSO. The focus of this work is introducing people to MOSO problems and give them a brief understanding of real-life representation of MOSO. The introduction to MOSO includes an overview of existing theory and some real life examples in agriculture, healthcare and logistics.

Is Hydrogen-based Steel making- The Future?

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Steel is the most cardinal pillar in this modern day scenario. It is an important aspect of our lives - the widely used engineering and construction material. Being one among the three largest producers of carbon emissions, the steel industry is under pressure to reduce its carbon footprints. On contemplating decarbonisation, hydrogen based steel making is being studied as one of the alternative methods. The changes required in the conventional method to achieve hydrogen based steel production and its challenges are discussed. This provides an overview of the process involved to gauge its feasibility and success to lead a sustainable future.

A Holistic Approach for the Model-based Control of Crystal Size and Purity in Integrated Continuous Crystallization-Wet Milling-Classification Systems

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Control of crystallization processes is essential to avoiding problems in the efficiency of downstream processes such as filtration and drying, and achieving the desired final product form (e.g., tablets). An important property of crystallizers is crystal size distribution (CSD). The shape and size of crystals affect the desired critical quality attributes (CQAs) of the final product, efficiency of the downstream processes, the compaction of the powder and the rate at which the human body absorbs the drug.

This study focuses on development and improvement of a one-dimensional model for process intensification and integration for active pharmaceuticals ingredients (API). For a uniform product, it is desired to have a narrow CSD minimizing the crystal size variation while for manufacturability it is desired to have bulky crystals. The former makes particles heavier and consequently less sticky while the latter decreases the dynamic and static friction between the particles and their environment consequently enhancing the flowability. Milling integrated crystallization systems are used due to the ease of use and safety, rather than screening and introducing new chemicals to the system as growth rate modifiers.

Crystallization is operated as batch, semi-batch and continuous processes. Although continuous processing is a common and established method in many industries, the pharmaceuticals industry has not yet fully embraced the technique and batch operation is still the most common approach for production. To affect the crystal size and shape distribution, mixed suspension mixed product removal (MSMPR) crystallizers are used in various configurations such as single-stage, multi-stage, with or without recycle streams, coupled with classifiers to separate fine particles from coarse crystals, etc. A good continuous crystallization process must achieve high product yield analogous to the current batch systems. One way to achieve this is with solid recycle, since it increases the surface area and hence the rate of mass deposition. A downside of recycle is however, the increase of impurity in the final solid product.

In this work, a model for a network of multi-stage continuous crystallizers connected to a downstream wet mill and two classifiers were developed and the effect of recycle on crystal size and purity was studied. An attainable region was found for crystal size and purity by optimizing the process for recycle ratio, wet mill's and classifiers' impeller speeds and crystallizer temperatures. A model was developed for tracking impurity in crystals and effect of recycle on impurity was investigated. It was found this framework resulted in isolating the CQAs and could be applied to other compounds without having to create separate design spaces. Also, uncertainties and robustness of the system were studied and the variables' effect on the dynamics of the system determined and a minimization for startup time, which leads to reduced cost and less wasted materials.

Extraterrestrial Habitat

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The potential existence of lunar lava tubes has been studied for over half a century. The improvement of high-quality image technologies became a great asset for space investigation facilitating the mapping and analysis of the Moon's surface. In addition to that, space explorers are reaching new territories with the help of advanced technology and engineering; the Mars surface is being explored, and the information collected is the first step towards bringing human life to the red planet.

Government agencies and now private commercial companies are carefully looking at the potential of space exploration. The Moon brings interest from different industries. Mining, science, tourism, possible water existence in the form of ice, and the ultimate goal of a permanent extraterrestrial settlement are among a few trend topics. The Moon is also strategically located between Earth and Mars, which could be helpful for future explorations of the red planet. However, it is necessary to protect future explorers against the Moon's hazards to accomplish this goal. The Moon has many inhospitable characteristics, but the most studied ones are the threats stemming from the lack of air pressure and oxygen, extreme temperature fluctuations, and hazards such as meteorite impacts and intense particle radiation.

Another Moon hazard is related to Moonquakes, and those are divided into four important categories. As previously mentioned, the seismicity from meteorite impacts, thermal quakes from contraction and expansion due to thermal differences of lunar materials, and deeper and shallow quakes. According to Nasa data from Apollo missions, shallow quakes have been registered only a couple of times. However, shallow quakes can be as strong as 5.0 on the Richter scale and could have a long duration compared with Earthquakes (Watters et al. 2019; science.nasa.gov) and could represent the biggest threat to a permanent human settlement on the Moon.

All those environmental threats on the Moon bring the necessity of human shelter. Building a shelter requires extra materials, and the transportation of those materials to the Moon can be incredibly costly. A good alternative is to use structures already existent in the lunar underground, the lava tubes. Like on Earth, lava tube formation occurs due to volcanic activity; after the eruption is ceased and the lava is not inside the tubes anymore, the underground structures remain available.

The stability of the lava tubes is the main point of this research. To use the lunar underground structures as human shelter, it is essential to evaluate how stable those structures are in the face of the Moon hazards. Numerical models and finite element analysis will be used for this evaluation. Data analysis is not concluded yet. For this symposium, the objective is to present the goals of this research.

Extraterrestrial Habitat, Moonquakes, seismic stability, lunar lava tubes

Blast Effects on Steel-Plate Composite (SC) Structures: Design for Direct Shear

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The design for blasts and explosions on structures is critical given the increase in terrorism, war and advanced weapon systems seen in the 21st century. Conventionally, reinforced concrete structures have been used in protective structure applications; however, steel-plate concrete composite structures (SC) have been offered as a viable alternative in many nuclear and defense applications. The SC wall section involves a concrete core between two steel plates. Steel reinforcement includes shear stud anchors and tie bar reinforcement, confining the concrete and allowing for ease of construction and modularity. Current protective structures are designed for blast loads in the structure's flexural response which sees a ductile response and large displacements. However, blast loads of high pressure in short duration can also produce an early shear failure before the desired flexural response. This failure, known as direct shear, can lead to a sudden collapse of the structure. This presentation will provide an overview of SC blast behavior with a design focus on direct shear. The current findings of ongoing work including full scale static direct shear beam testing, numerical modeling and design tools will be discussed. This research addresses the large gap in the profession on direct shear, especially direct shear in SC. Proper direct shear design is imperative for protective structures so the structure can have the appropriate level of blast protection. Including the direct shear failure mode in SC only leads to an increase in the survivability of personnel, assets and critical structures.

Representing Multiple in vitro Tuberculosis Infection Models with a Single in silico Agent-Based Model

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In vitro methods are commonly used to study host-pathogen interactions in M. tuberculosis (Mtb) infection. There has been a recent interest in developing spheroid models that can represent the TB granuloma environment more closely than the traditional (trad) cell culture plate counterparts. Previous work has shown that spheroid models using PBMCs have better bacterial control than trad culture equivalents, but the cause of these differences is unclear.

We use an in silico model to simulate both spheroid and trad culture to explore whether the difference in Mtb control can be solely due to spatiality. An agent-based model is constructed with Mtb, macrophages (Mϕ), CD4+ and CD8+ T cells. Mechanisms include phagocytosis of Mtb by Mϕ and activation of Mϕ through NFκB and STAT1. Parameters include secretion rates, activation thresholds, and probabilities of killing and movement. After a large parameter sweep using latin hypercube sampling, we select parameter sets that fell within the experimental Mtb counts and sampled ranges around these to enrich sets that represent the entire experimental range.

Our results suggest that spatial differences alone can account for the differential Mtb control. Preliminary results suggest that poorer Mtb control in the trad model is due to lower levels of Mϕ activation. Notably, the spheroid model has more activation of infected Mϕ. The difference in infected Mϕ activation is specifically due to STAT1, implying more T cell activation in the spheroid model. But the opposite was seen, with trad model having more activated T cells.

Together, our results suggest that the spatial organization of spheroids allows for more targeted, effective T cell activation. Our model can be used to answer further hypotheses about the dynamics of early Mtb infection in granulomas and to possibly “3-dimensionalize” the results of trad in vitro models.

An Optimization Framework for Distributed Manufacturing of Electrified Chemical Processes

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Chemical industries are a major source of greenhouse emissions as they are powered mostly by the combustion of fossil fuels. To solve this problem, electrification of the chemical industry is a solution that is currently being explored by researchers across the world. Electrification helps decarbonize the chemical industry and transition from fossil fuels to more renewable energy sources such as solar and wind. The main challenge of transitioning to renewable-based energy is that their output varies across locations and different time scales. Millions of dollars might be saved if electrified processes can be designed to adapt to these variations. Therefore, there is a need to model both the detailed temporal and spatial features for electrified chemical processes and integrate the planning of the power resources with the chemical processes to implement electrification throughout the industry. This project will help address this gap by considering three-time scales, single-time, monthly, and hourly, as well as the spatial variations in co-planning chemical processes and power networks using the concept of "Distributed Chemical Manufacturing (DCheM)". DCheM is a concept that aims to improve chemical process industries by developing modular process plants and taking advantage of distributed resources and/or addressing distributed environmental problems as well as reducing transportation costs.

To model the problem, an MILP (Mixed Integer Linear Programming) model is proposed for locating and designing modular electrified plants operating in different modes, renewable power generating units and transmission lines in candidate locations of a network that integrates optimized planning and scheduling of these different components. The proposed model has three-time scales which include single-time investment decisions, monthly decisions, such as transportation of chemicals to meet customer demand, and hourly decisions, such as chemical production and power flow. Integrating planning and scheduling in a single model leads to many variables. To solve the model efficiently, the model must be decomposed. Thus, appropriate decomposition models must be proposed.

Till now, we have tried solving this problem on a small scale considering 5 candidate locations coordinated by a microgrid. We proposed a bi-level decomposition algorithm and adapted the Lagrangian decomposition algorithm to solve the model efficiently with different monthly demand profiles. The power of decomposition algorithms is such that the right decomposition algorithm when applied can reduce the time taken to solve the model considerably. For instance, the proposed bi-level decomposition algorithm, for a particular demand profile obtains a solution to the problem within 4.2% time of solving the MILP model without decomposition and obtaining a similar solution while maintaining an optimality gap of 0.042%. The models and algorithms obtained through the project will help plant owners with the planning of different components and scheduling of their operations for the effective implementation of electrification throughout the entire chemical industry. In the future, we would like to extend this model to have more candidate locations and integrate the central planning of the U.S power grid.

Sensing and Memory via Engineered Materials

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As structures become more advanced and responsive, they require increasingly advanced sensing capabilities. For example, adaptive airplane wings require sensing across the area of the wing to respond to changing aerodynamic conditions, and robots need vast arrays of sensors to detect unstructured environments. This large area sensing can result in an overload of data for on-board computers, which are unable to read, process, and respond to such a large amount of sensor data without buffering delays or memory shortages. One solution to maintain large area sensing capabilities, while minimizing the required digital processing, is to use mechanical sensors, commonly referred to as mechanosensors. Mechanosensors leverage the mechanical properties of the sensor itself to sense and record external stimuli.

We develop an engineered material, or metamaterial, to sense external force patterns using mechanosensing. This presentation will describe how we use the material and structure of dome-shaped unit cells to achieve mechanics-based sensing of external forces, rather than relying on conventional digital sensing. Each dome is bistable, meaning it is stable in both popped-up and popped-down configurations, with a minimum force input required to change configurations. This bistability gives the metamaterial two key mechanosensing capabilities: inherent filtering of external signals below a certain force threshold and nonlinear amplification of signals above this threshold. We then link these unit cells to memristors, a special type of resistor which changes resistance over time in response to repeated triggers. The memristor readouts may be fed into a simple neural network that allows us to retrieve force patterns experienced by the metamaterial. The demonstrated capability of the metamaterial to sense and remember external force patterns entirely through its mechanical properties, without the use of conventional digital processing, has important implications for many engineering fields, including aerospace, robotics, and packaging.

Enhancing Thermal Conduction in Polymers

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Higher power densities and consumption in electronic devices require heat dissipating components with high thermal conductivity to prevent overheating and improve performance and reliability. Polymers offer advantages of low cost and weight over metallic cases, but their intrinsic thermal conductivity is low. Previous studies have shown that the thermal conduction in polymers can be enhanced by polymer chain alignment or by adding high thermal conductivity fillers to create percolation paths inside the polymeric matrix. Typical thermally conductive polymers have moderate in plane conductivity, but low cross plane conductivity. The cross plane thermal conductivity is critical to removing heat from active devices and transmitting it to the external environment. In this study, we combine strategies of past work leveraging conductive fibers and fillers to enhance thermal conductivity of polymers without inducing significant thermal anisotropy. We fabricate our thermally conductive polymer composites by infiltrating para-aramid chopped fiber mats with an epoxy matrix. We then characterize the mechanical performance of the composites with different stiffnesses and curing accelerant concentrations by performing cyclic loading experiments in a dynamic mechanical analyzer (DMA). For the thermal characterization, we use infrared thermal microscopy with two different experimental set ups that allow us to obtain values for the in plane and cross plane thermal conductivity independently. We show that by tuning the stiffness of the polymeric matrix we can produce composites with different mechanical properties applicable for a range of applications in the electronics industry. The results also show that the network structure achieved by the fiber mat allows a uniform increase in the thermal conductivity of the composite in all directions. Future work will evaluate metallic or carbon-based fillers in combination with the fiber mats to achieve even higher thermal conductivity in these composites.

Transitions in the Workflow of a Psychiatric Unit During the COVID-19 Pandemic and Design Implications

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As in many other aspects of society, the COVID-19 pandemic imposed a stress test on the entire healthcare system. Hospitals faced complex challenges, including making adaptations to each unit's specific characteristics and needs. Inpatient psychiatric units differ substantially from other hospital units, creating unique problems and considerations to safely manage patients, families, and healthcare staff during a pandemic. As research is done to improve our infrastructure for future pandemics, facilities with psychiatric units have unique design considerations. This thesis aims to examine the effects of the COVID-19 pandemic on the workflow of a psychiatric unit and its possible implications on future design requirements. Specifically, looking at transitions, i.e., what areas remained unchanged, what changes were made but have not persisted, those that persisted, and what needs to be improved to better function in the next pandemic. The methodology used in this study included an examination of current design requirements and specifications and the workflow in a facility of this type. To maintain the facility's and staff's privacy, the specific unit is identified as Unit-A. A construction firm provided access to drawings, and engineers were interviewed to elucidate specific design/performance requirements. The methodology also included interviews of nurses and administrative staff actively engaged within Unit-A throughout the pandemic. A workflow was established based on the information collected before and during the pandemic. An analysis of the interviews and the workflow revealed: (i) the highest demands were placed on the direct-care staff, and (ii) policies implemented by the hospital without special consideration for the psychiatric unit caused unintended strain on the workflow. These significant findings suggest that each hospital should have a unique pandemic plan to accommodate their respective units and be designed with more multipurpose/convertible space to allow for more flexibility within the infrastructure of the unit. Obtaining more input from those directly impacted will improve the resiliency of the workflow. These findings also suggest that design specifications need to more effectively incorporate the needs of the professional staff, such as including a larger number of spaces for the healthcare staff in the hospital compared to current standards

Silicon Carbide MOSFET and the era of sustainable electrification

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Roughly one-fifth of all CO2 emissions in the US is contributed by vehicles. Reducing CO2 emission is one of the key challenges in the 21st century in addressing climate change. The electrification of vehicles provides the sweet spot between climate concerns and comfort. Following the footsteps of Tesla- the leading electric vehicle (EV) manufacturer, renowned companies like General Motors, Ford, etc. are investing billions towards reducing vehicle carbon footprint and going all electric soon. Soon EVs will be as ubiquitous as SUVs. With the right technology, the EVs can be charged fully in roughly same amount of time as it takes to fill the gas tank of SUVs. One such technology is the emergence of Silicon Carbide (SiC) Metal Oxide Semiconductor Field-effect Transistor (MOSFET) application in EVs. MOSFETs, or in the simplest term – transistors - are the fundamental building blocks of electronic devices.

SiC is a wideband-gap semiconductor material with superior properties that makes it a favorable candidate for application in EVs and high-power applications in the silicon (Si) dominant industry. Our research involved the design, simulation, and fabrication of novel vertical SiC power MOSFETs, rated at 650V - 900V, capable of withstanding operation temperature up to 200° C, over and above the operating range of Si. Figure of merit of SiC power MOSFETs is specific on-resistance and blocking voltage. IMOSFET- our vertical SiC power MOSFET has highly scaled trenches etched into the substrate that look like letter "I". These trench structures increase the effective width of the current-carrying regions without increasing the device area, i.e., more devices can fit on a single wafer, bringing down the cost of SiC power MOSFETs. With these structural innovations, the specific on-resistance of IMOSFET is 12X lower than commercially available SiC MOSFETs with a 6X lesser cell-pitch (device area).

The size of MOSFETs is especially of concern in the power control unit (PCU) of EVs. The space available in EV engine compartments is often very limited that PCUs with compact design and higher power density are desired. The IMOSFET is designed for exactly the same purpose. At 1200 volts, a SiC IMOSFET module can have a die size 20X smaller than its comparable Si part at a reduced cost. In 2020, Tesla Model 3 sedans alone put 9 million SiC MOSFETs on the road. As the automotive industry progresses toward electrification, it is expected that by 2035, there will be more than 2.4 billion 650V SiC MOSFETs brought on road every year. To meet such an enormous demand, faster and affordable manufacturing of SiC MOSFETs will be a must. Our research in vertical SiC MOSFETs sets a solid ground for affordable electric vehicles to evolve, flourish, and reach their highest performance potential in the near future.

Criteria Development to Assess Pack-out Corrosion Effects in Steel Built-up Members

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Pack-out or pack-rust corrosion is a localized rust found between steel plates. This type of corrosion affects built-up members, especially old bridges. Pack-rust is unlike other corrosion because it induces local distortion to the structural members, where no displacement is expected. Unfortunately, the corrosion changes how the connection between steel members interact, as well as the stability of the structure, but its effects are poorly understood. This project aims at describing the effect of pack-out corrosion on steel members under compression forces. The goal is to reliably evaluate structures that are still in-service to determine if the pack-rust corrosion requires maintenance.

Experimental studies were performed to test the fatigue life of steel members under compression with pack-out. The fatigue analysis was conducted via cyclic loading on the beam. This was done to determine if failure would occur either locally, via a crack, or globally, via complete failure of the member. Additionally, a strength test was performed on similar samples. Results showed pack-rust corrosion affects yield strength and maximum capacity of the member, while minimally affecting the member's stiffness. The shape of the steel member, rust formation, forces applied, deformation and stresses were recorded and used as benchmarks for modeling these tests on a finite element analysis (FEA) software (ABAQUS).

Experimental data matches the analytical results, demonstrating the reliability of this novel FEA model for the first time. It allows for further investigation of variables affecting built-up steel members under compression loading. In particular, a significant factor affecting the pack-rust formation and the capacity of the old steel member are the shape of the built-up member, the type of fasteners (rivets or bolts), and the method of attachment (straight, staggered, pre-tensioned, or post-tensioned). Further research is needed to refine the model such that it becomes a useful field tool for recommendation of maintenance.

Multi Modal Drug Delivery Platform for Functional Restoration of Spinal Cord via White Matter Repair

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Therapeutic targeting of the spinal cord has been challenging to resolve due to the dynamic relationships and synergistic processes making up tissues in the central nervous system (CNS). Due to the complex architecture and diversity of tissue, targeting a degenerative process, such as demyelination, in isolation will not yield significant progress toward potential modalities of clinical treatment for spinal trauma. Combinatorial drug delivery strategies are a promising avenue to approach functional restoration due to their capacity to be tailored to specific symptoms and engineered to respond to inflammation in a cascade. This prompts the design of a platform that can pass the blood brain barrier, adhere to selective tissue surfaces, and sequentially release active compounds for therapeutic effect. This is done through polyethylene glycol (PEG) based micelles that can be grafted with carboxylated ethyl cellulose to form a multi armed macromolecule that is polyphilic and biocompatible. In the context of functional restoration of the spinal cord, particularly after accelerated impact, focusing primarily on white matter narrows down the pharmacological needs of demyelinated axons, poor signal conduction, and secondary inflammation of non-impacted tissues. The macromolecule has toll-like receptors coating the micelle surface to allow for selective binding to macrophages en route to a site of injury. The cascade-inducing compounds are tagged and consist of a potassium channel blocker, an immune modulator, and an antioxidant. The study is divided into three phases: in vitro, in vivo, and ex vivo. The models used in the study elucidate distribution patterns of anti-inflammatory activity as well as associated changes to neural structure after a 12 week period, during which secondary injury is expected to be in the chronic phase when scar tissue formation takes place, sterically hindering new tissue growth. The in vitro phase of this study will demonstrate the efficacy of drug shuttling and release. The experimental strategy in vivo involves the administration of the macromolecule in a saline media directly into the spinal white matter. Anisotropic flow of solution is expected due to the fibrous structure of white matter. Ex vivo analysis is where conduction speed quantification can take place using double sucrose gap junction recording. The results of this study will encourage further investigation into customized pharmacological treatments that may eventually translate in human clinical trials and offer a functional recovery of crucial tissues even over a length of time.

Process Intensification of Energetics Crystallization via model-free Quality-by-Control Direct Design Approaches

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Crystallization is an essential process of solids manufacturing and is left unoptimized in several fields, including energetics manufacturing. Unoptimized crystallization protocols can lead to particles with undesired physical and chemical characteristics, such as particle morphology, sensitivity, detonation potential, manufacturability, and overall crystal quality. First manufactured for use in World War II, nearly a century ago, Research Department/Royal Demolition Explosive (RDX) and High Melting Explosive (HMX), have been applied to military munitions, propellants, and general explosives and continue to be two of the largest manufactured energetic materials. Although researchers have extensively studied the solubility of the common energetic materials, RDX and HMX, little work has been completed on the process intensification of RDX and HMX crystallization.

In this work, we demonstrate the combination of model-free Quality-by-Control (mf-QbC) and model-based digital design to develop a robust process intensification framework for the crystallization of energetic materials. mf-QbC allows for the minimization of experiments and exposure by utilizing feedback control strategies for desired critical quality attributes (CQAs) (Simone et al., 2015). Small-scale experiments completed with Crystalline showed that RDX and HMX have high solvent power (solubility) in γ-Butyrolactone and good temperature sensitivity which is desirable for crystallization control. The two applied direct design approaches are direct nucleation control (DNC) and supersaturation control (SSC). DNC uses particle counts measurements collected with an in-situ focused beam reflectance measurement (FBRM) probe in a model-free closed feedback control approach, which introduces temperature cycling, stimulating controlled nucleation and crystal growth (Bakar et al., 2009). SSC uses solution concentration measurements collected with an in-situ infrared (IR) probe in a model-free closed feedback control approach that drives the temperature profile to maintain constant supersaturation (Saleemi et al., 2012). In application with in-situ process analytical technology (PAT) tools, DNC and SSC allowed for the selection of crystallization design parameters that control the desired CQAs of RDX and HMX and the further optimization of the selected design parameters via model-based digital design. Intensifying the industrial crystallization of common energetic materials, such as RDX and HMX, will improve the quality of manufactured energetic materials, and future process development for the manufacturing of energetic materials.

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Physics Informed Neural Networks to reduce uncertainty in experimental measurements

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A metrology tool based on 2D Laser Angstrom Method has been developed for the characterization of anisotropic thermal conductivity in the in-plane direction for thin material sheets. While the experimental setup enables us to obtain the Infrared thermal data, a data-processing algorithm is needed that processes the given data and predicts the values of the thermal properties. The existing post-processing technique involves applying least squares fitting method to obtain the necessary predictions. However, due to noise in the experimental data, a certain level of uncertainty is introduced in the measurements. Our goal is then, to minimize the error in the predictions by incorporating high-accuracy computational algorithms. One of the promising ones is Physics Informed Neural Networks (PINNs). These are a method used to solve ordinary and partial differential equations (ODEs and PDEs). They combine the computational advantages of the machine learning algorithms with the universality of the underlying Physics governing differential equations, to predict the values of thermal conductivity efficiently and accurately. The general PINNs model consists of a neural network with a specific architecture (the number of hidden layers and the number of neurons in each layer) which is trained using the temperature data that we obtain from our experiments. This trained neural network works in combination with the governing equation (of 2D in-plane transient conduction) to reduce the difference between the expected and the predicted data values. By appropriately tuning our model parameters (network architecture and weight losses), we show that we can accurately predict the thermal properties of the materials of concern.

Viability of Focused Ion Beam Milling to Machine Crystalline Explosives

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HMX single crystals are particularly difficult to machine due to their brittle, delicate nature. As such, effective machining methods are limited. Previous research has focused on the impacts of cylindrical pores created by drilling or by using the drill press to mill slots to mimic large cracks, both methods limiting pore shape and introducing preliminary mechanical stresses. The Focused Ion Beam (FIB) uses accelerated ions to sputter away material, which when coupled with the light elements that comprise HMX make milling relatively large depths (mm range) possible. Additionally, FIB allows for increased milling dimension control and the ability to form sharp corners that were previously unattainable. Pores with greater complexity and control may be generated as well as, and more importantly, in variable geometries that better mimic naturally occurring flaws.

Assessment of Innovative Repair Methods for Corroded Steel Girder Bridges Using House of Quality Matrix

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Across the United States, steel girder bridges experience significant corrosion damage: 7% out of 617,000 steel bridges across the country are considered structurally deficient as per a recent estimate. Current repair procedures for corroded steel girder bridges, such as (i) Replacing Corroded Parts by Welding and (ii) Bolting Angle Sections or Steel Plates, require considerable time and budget. Therefore, there is a need for cost-effective, rapid, and robust repair strategies that can be implemented by bridge maintenance personnel. This paper presents five modern repair methods for rehabilitating corroded steel girder bridges: (1) Encasing the Corroded Part with UHPC (Ultra-High Performance Concrete) (2) Strengthening the Corroded Part with CFRP (Carbon-Fiber-Reinforced Polymers) (3) Double Steel Plates Filled with Cementitious Material ("Sandwich Panel") (4) Improved Bolted Angle Method (5) Strengthening the Web with Diagonally Oriented Angle.

The five repair methods were evaluated to select two repair methods that can be further implemented by the local DOT (Department of Transportation) in Indiana. During the evaluation process, many requirements associated with repair methods for corrosion-damaged steel girders were considered, including robustness, reduction of implementation cost, and construction time. In addition, feedback from the local department of transportation in Indiana (INDOT) was collected to further identify any additional requirements. A House of Quality Matrix (HQM), a commonly used tool in the consumer product industry, was used to choose two repair methods for further development. After completing the evaluation, "Sandwich Panel" and "Strengthening Web with Diagonally Oriented Angle" repair methods were selected.

This paper will discuss innovative repair methods, HQM as a tool, and anticipated future work including destructive testing of decommissioned bridge girders with implemented repair techniques. On top of that, numerical investigations will be conducted, and detailed guidelines on designing the repair for two Innovative Repair Methods will be created.

Paper-based Lateral Flow Immunoassay for HPV Protein Detection

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Among women globally, cervical cancer was the fourth most common cancer in 2018 with an estimated 311,000 deaths reported [1]. Approximately 85% of these deaths occurred in low-and middle-income countries (LMIC) due to limited access to medical resources. In response, the World Health Organization called to action the elimination of cervical cancer through global implementation of two preventive interventions: human papillomavirus (HPV) vaccinations and early screening [2]. A large majority of cervical cancer (>95%) is due to HPV; however, vaccines are not readily available in LMIC. Over the next 50 years, an estimated 60% of cervical cancer cases can be prevented using improved screen-and-treat strategies alone [3]. Unfortunately, current screening technologies cannot combine highly sensitive and specific detection with single-visit, signal readouts detecting HPV at the point of care (POC). Here we generate prototypes for scalable manufacturing and user-centered design of a lateral flow immunoassay (LFIA) to detect HPV with our partners in Zambia.

The LFIA was developed to detect HPV16 L1 capsidic protein, where its under-expression is associated with an increased degree of cervical lesions [4]. To target L1 proteins, an anti-HPV16 L1 detector antibody was conjugated to gold nanoparticles (AuNP) to qualitatively observe the protein-antibody binding. The L1 protein concentration was varied (10-891 ng/mL) to identify the lowest limit of detection (LoD). Dot blot microassays were utilized to confirm the protein-antibody binding and LoD. Pictures were taken of the dot blot results before ImageJ analysis provided the signal intensity.

The LoD for L1 proteins was reliably detected at 50 ng/mL. The dot blot results provided further insight into the clinically-relevant concentration range needed to translate these findings towards the fabrication of LFIA prototypes. The design and fabrication of these LFIAs will guide the device's sensitive detection to HPV16 L1. Future work focuses on adopting automated striping and assembly for rapid, scale-up production and device performance testing. Upon optimization, this POC diagnostic device will be used for early screening of cervical cancer risk from HPV infection.

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Enzymatically Signal Enhanced Lateral Flow Assay Test for HIV using p24

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In 2020, an estimated 1.5 million people had contracted HIV globally. Of that, approximately 84% of those living with HIV knew their status. The remaining 16% (about 6.0 million people) are unaware of their infected status and require HIV testing [1]. HIV testing is a critical first step in HIV prevention, treatment, care, and support hence there is a need to develop a quick, easy, and cost-effective point-of-care test for HIV detection. The time between HIV infection and a detectable HIV antibody concentration can be up to 90 days. By incorporating more sensitive testing for the HIV p24 antigen, the window time can be reduced to 17 days [2]. Additionally, using a signal enhancement technique, that window can be further shortened, making it easier to detect acute infection. This work focuses on developing an enzymatically signal-enhanced lateral flow assay test using the p24 antigen to detect HIV during the acute phase. An octet biolayer interferometry instrument was used to screen a set of 8 antibody pairs for rapid binding kinetics and strong equilibrium binding to p24 antigen, both of which are required for lateral flow assays. The dot blot technique was then used to assess and enhance the functionality of the individual components used in the development of the lateral flow assay test. The antibodies were screened based on a visual color gradient formed by protein coupled with antibody-conjugated gold nanoparticles and a quantitative analysis was performed using ImageJ software through signal pixel intensity analysis. A limit of detection of 78 ng/mL was obtained for detection of p24 antigen in the patient sample. This limit of detection was improved to 0.76 ng/mL by using AuNP-Ab conjugates with horseradish peroxidase (HRP) enzyme which converts the colorless diaminobenzidine substrate to a deep brown precipitate for enhanced detection and better interpretability [3]. Additionally, a dipstick method was used to examine a semi-assembled lateral flow test to gain insights into the fabricated components and flow properties of the test. Future work includes continuing to optimize the antibody-antigen binding using dotblot and dipstick methods to further lower the limit of detection and integrating the lateral flow test into an automated fluid delivery system. Upon optimization, this point-of-care diagnostic device will be used for early detection of HIV to help attain UNAIDS's goal to end AIDS as a public health threat by 2030.

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Atomistic view of metallic systems

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Superalloys are most notably used in jet turbine engines. The high temperature and high strength demand of this application require innovative solutions for advancement. It is understood that a 1% increase in efficiency, achieved through increasing operating temperature and strength, results in $66 billion in fuel savings over 15 years.

My research focuses on a phenomenon called local phase transformation (LPT) strengthening. Before explaining this phenomenon in detail, it is important to understand that metals are crystalline materials. Meaning, they have a very distinguished planar atomic packing sequence (imagine a stack of oranges). Additionally, metals deform through dislocations. You can think of a dislocation in this way: if you imagine moving a large rug, it would be difficult to move the rug by pulling one corner because the friction of the rug is great. Alternatively, if you move the rug in a way similar to a caterpillar-- creating a bubble and sliding the bubble through, the rug will move much easier. In the same way that it would be difficult to overcome the friction of a rug by pulling one corner, it would be difficult for the material to break all its bonds on a plane. Material strength comes from the impedance of dislocations.

My work focuses on a complex dislocation deformation mechanism called a stacking fault. Stacking faults are unique because while a single-phase material has one stacking sequence, upon deformation across 4 atomic planes, the stacking sequence changes. This creates a high energy fault. To lower the system energy, elements (Ti, Ta, Nb - in my case) segregate to these high energy faults. Where this change in structure and segregation of elements occur, a “local phase transformation”forms. Secondary phases are important because of how they impede dislocation motion. Continuing with the rug analogy, given an immobile point (small table) in the middle of the rug, the dislocation bubble would stop. While there are other ways to impede dislocations, it is common to design metals with secondary phases. This design property (secondary phases) is usually done in the bulk of the material and is not induced upon deformation. This idea encapsulates how my work is different. We are designing a specific composition of alloys that create an atomic secondary phase as they deform. As to say, while the material is deformed it becomes even stronger. In practice, I leverage computational resources to design alloy compositions, make the alloys, mechanically deform them, and quantify segregation and strengthening.

Local phase transformation strengthening has only recently been discovered and alloy design efforts to optimize and quantify the mechanism are not well understood.

Liquid flux assisted growth mechanism for the chalcogenide perovskite- BaZrS3

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Chalcogenide perovskites are emerging photovoltaic materials with attractive optoelectronic properties including a high absorption coefficient, tunable bandgap, and high dielectric constant. In contrast to their halide counterparts, these materials have been shown to be stable, and earth-abundant with nontoxic constituents. However, the current rudimentary synthesis techniques have limited the growth of these materials. Traditional solid-state and vacuum processing methods demand temperatures in excess of 800-1000°C bringing up difficulties in identifying suitable substrates and subsequent device fabrication. Hence, gaining insights into the growth mechanism of these materials becomes integral for engineering robust fabrication methodologies.

To address this, we systematically studied the growth mechanism of the BaZrS3 perovskite through our earlier reported hybrid precursor route utilizing barium thiolate and zirconium hydride precursors. Preliminary findings demonstrate that the high-temperature requirements are related to mass transfer barriers between precursors rather than thermodynamic limitations. We also identified an accessible liquid phase capable of overcoming these diffusional barriers and driving the reaction towards lower temperatures as well as assisting in grain growth.

In conclusion, this work is focused on understanding the growth mechanism of the BaZrS3 perovskite and identifying the potential liquid phase to drive low-temperature synthesis and support subsequent thin film fabrication.

Roll-to-Roll Manufactured MoS2-Carbon Nanotube Sensors for Selective Detection of Acetone

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Recently, the detection of volatile organic compounds (VOCs) showed significant potential in environmental toxicological analysis, early diagnosis of diseases, detection of crop-relevant pathogens, and food quality control. Two-dimensional materials have been widely applied to VOC detection because of high surface-to-volume ratio, which provides highly active surfaces for molecular adsorption. Among all 2-D materials, molybdenum disulfide (MoS2) stands out with its excellent electronic properties, environmental stability, and mechanical properties. Exhibiting these advantages, MoS2 provides great potential for high-performance electronics and sensors-related applications. In this work, a fully roll-to-roll (R2R) manufactured chemiresistive MoS2 and single-walled carbon nanotube (SCNT) sensor for VOC detection has been developed. The MoS2-SCNT sensor is based on flexible, screen-printed silver interdigitated electrodes (IDEs), on which exfoliated MoS2 suspension and SCNT suspension were electro-sprayed in sequence. Through alternate spraying of these two materials, the layer-by-layer spraying resulted in a nanohybrid structure exhibiting optimal sensitivity. According to the microstructural surface characterization, Scanning Electron Microscopy (SEM) images demonstrated the nanoporous structure which proved beneficial for gas adsorption. In Transmission Electron Microscopy (TEM) images, the carbon nanotubes served as channels electrically connecting the MoS2 nanosheets, which enhanced the charge carrier transfer, resulting in sensitivity and conductivity being greatly increased. To enhance the selectivity of the sensor to acetone, one of the most common VOCs, the functional group, tetrafluorohydroquinone (TFQ), was introduced. The hydroxyl groups on TFQ have high affinity to interact with acetone, so the selectivity to acetone can be increased. The experimental results showed that the response of acetone is linearly increased with respect to TFQ, which further proved the enhancement of sensor selectivity. In summary, we proposed an entirely R2R manufacturing method to fabricate MoS2-SCNT VOC sensors with high sensitivity, excellent selectivity, cost-effectiveness, and ease of fabrication. This platform shows great potential in applying various kinds of 2-D materials and nanomaterials to mass production, which is expected to have strong prospects in agriculture, the food industry, early diagnosis of disease, and environmental protection.

Deep learning driven adaptive optics for single molecule localization microscopy

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Single molecule localization microscopy (SMLM) forms super-resolution images with a resolution of several to tens of nanometers, by detecting isolated single molecule emission patterns and localizing the centers of individual probes. However, the inhomogeneous refractive indices distort and blur single molecule emission patterns, reduce the information content carried by each detected photon, increase localization uncertainty, and thus cause significant resolution loss, which is irreversible by post-processing. To compensate tissue induced aberrations, conventional sensorless adaptive optics methods rely on iterative mirror-changes and image-quality metrics to compensate aberrations. However, these metrics result in inconsistent, and sometimes opposite, metric responses which fundamentally limited the efficacy of these approaches for aberration correction in tissues. Bypassing the previous iterative trial-then-evaluate processes, we developed deep learning driven adaptive optics (DL-AO) for SMLM to allow direct inference of wavefront distortion and near real-time compensation. Our trained deep neural network (DNN) monitors the individual emission patterns from single molecule experiments, infers their shared wavefront distortion, feeds the estimates through a dynamic filter (Kalman), and drives a deformable mirror to compensate sample induced aberrations. The method simultaneously estimates and compensates 28 types of wavefront deformation shapes, restores single molecule emission patterns approaching the conditions untouched by specimen, and improves the resolution and fidelity of 3D SMLM through brain tissues over 130 μm, with as few as 3-20 mirror changes.