APTEC

2023 GULF COAST POLYMER CONFERENCE

Keynote Speaker

DR. ELIZABETH KELLEY

NIST Center for Neutron Research

Keynote Speaker

DR. RONALD CASTELLANO

University of Florida

Patrick F. Taylor Hall, South Quad Drive,
Baton Rouge, LA

DEC | **2nd** | **2023**

LSU

EVENTS SCHEDULE

APTEC

The Applied Polymer Technology Extension Consortium was originally created by an act of the Louisiana Legislature as a university-affiliated, 501(c)(3) not-for-profit, state-sanctioned engine of economic development, research, teaching and outreach. APTEC now enjoys all the freedom of any other non-profit and combines the physical and human resources of polymer-strong universities along the Gulf Coast. Unlike a government bureaucracy, APTEC operates at the speed of business. Universities benefit as APTEC scientists mine great ideas for long-term, fundamental study. APTEC provides swift and expert evaluation of intellectual property potential. APTEC is also engaged in community improvement and development of a new generation of entrepreneurs.

8:30 am-9:00 am (Capstone Gallery):
Registration, Breakfast, & Poster Setup

9:00 am-9:15 am (PFT 1100):
Introductory Remarks: Gulf Coast Polymer Conference Planning Committee

9:15 am-10:00 am (PFT 1100): Keynote Speaker: Dr. Elizabeth Kelley

10:00 am-10:15 am (Capstone Gallery): Coffee/Tea Break

10:15 am-11:45 am (PFT 1100, 1202, & 1259): Oral Presentations Session I

11:45 am-1:00 pm (The Commons): Lunch Break

1:00-2:30 pm (PFT 1100, 1202, & 1259): Oral Presentations Session II

2:30 pm-3:15 pm (PFT 1100): Keynote Speaker: Dr. Ronald Castellano

3:15 pm-4:15 pm (Capstone Gallery): Poster Session and Coffee/Tea

4:15 pm-4:45 pm (PFT 1100): Career Panel

4:45 pm-5:15 pm (PFT 1100): Key Principles of Visual Communication Design: Quynh Do

5:15 pm-5:45 pm (PFT 1100): Resume Workshop: Your Professional Brand: Marlo Milton

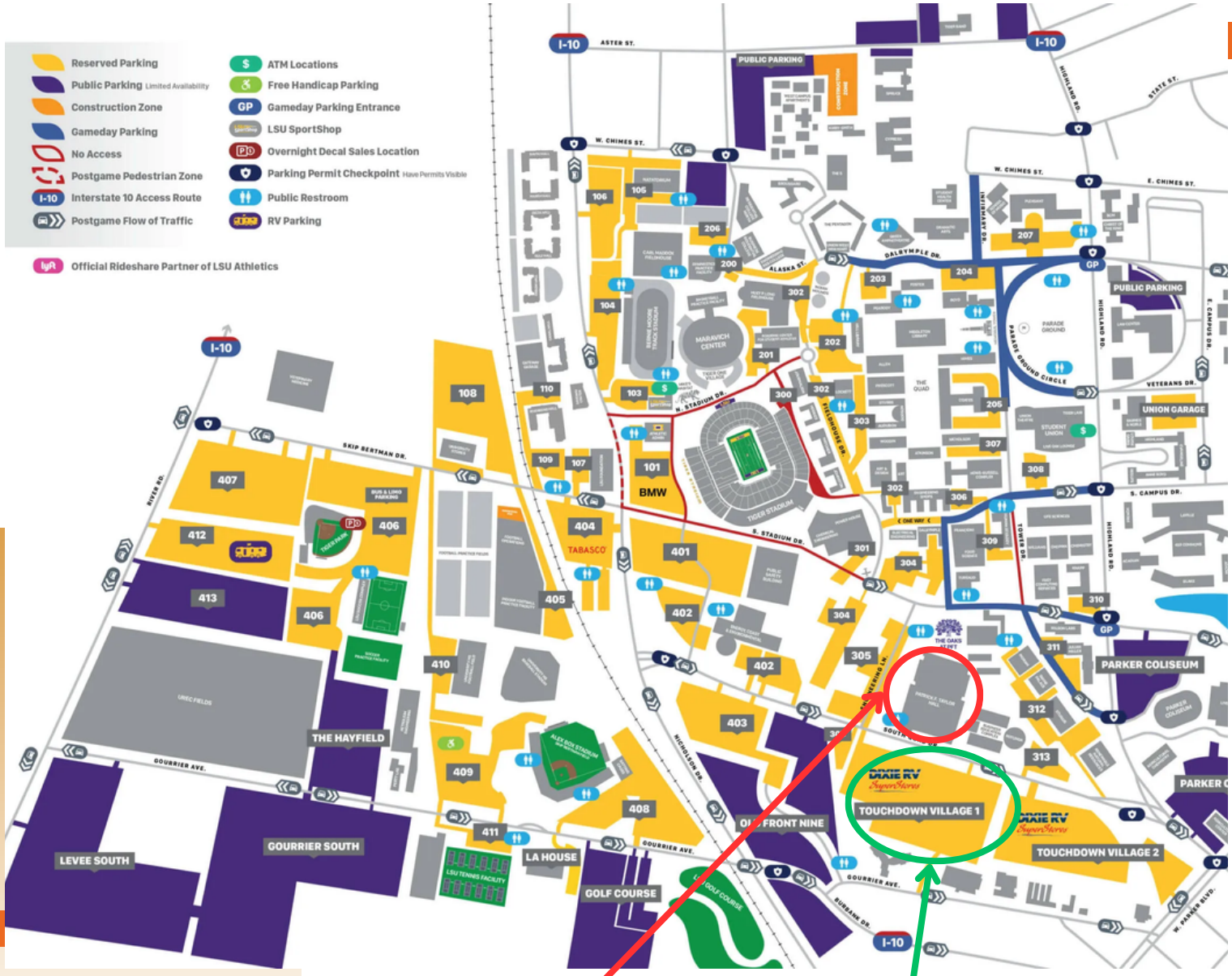
5:45 pm-6:00 pm (PFT 1100): Closing Remarks: Gulf Coast Polymer Conference Planning Committee

6:00 pm-7:00 pm (Capstone Gallery): Networking & Discussion

Gulf Coast Polymer Conference

LOCATION: PATRICK F. TAYLOR HALL; LOUISIANA STATE UNIVERSITY

LOCATION: PATRICK F. TAYLOR HALL; FIRST FLOOR (LOUISIANA STATE UNIVERSITY)
ADDRESS: 3304 S Quad Dr, Baton Rouge, LA 70803
PARKING: TOUCHDOWN VILLAGE 1 (ACROSS FROM PATRICK F. TAYLOR)



PATRICK F. TAYLOR HALL

PARKING (TOUCHDOWN VILLAGE 1)

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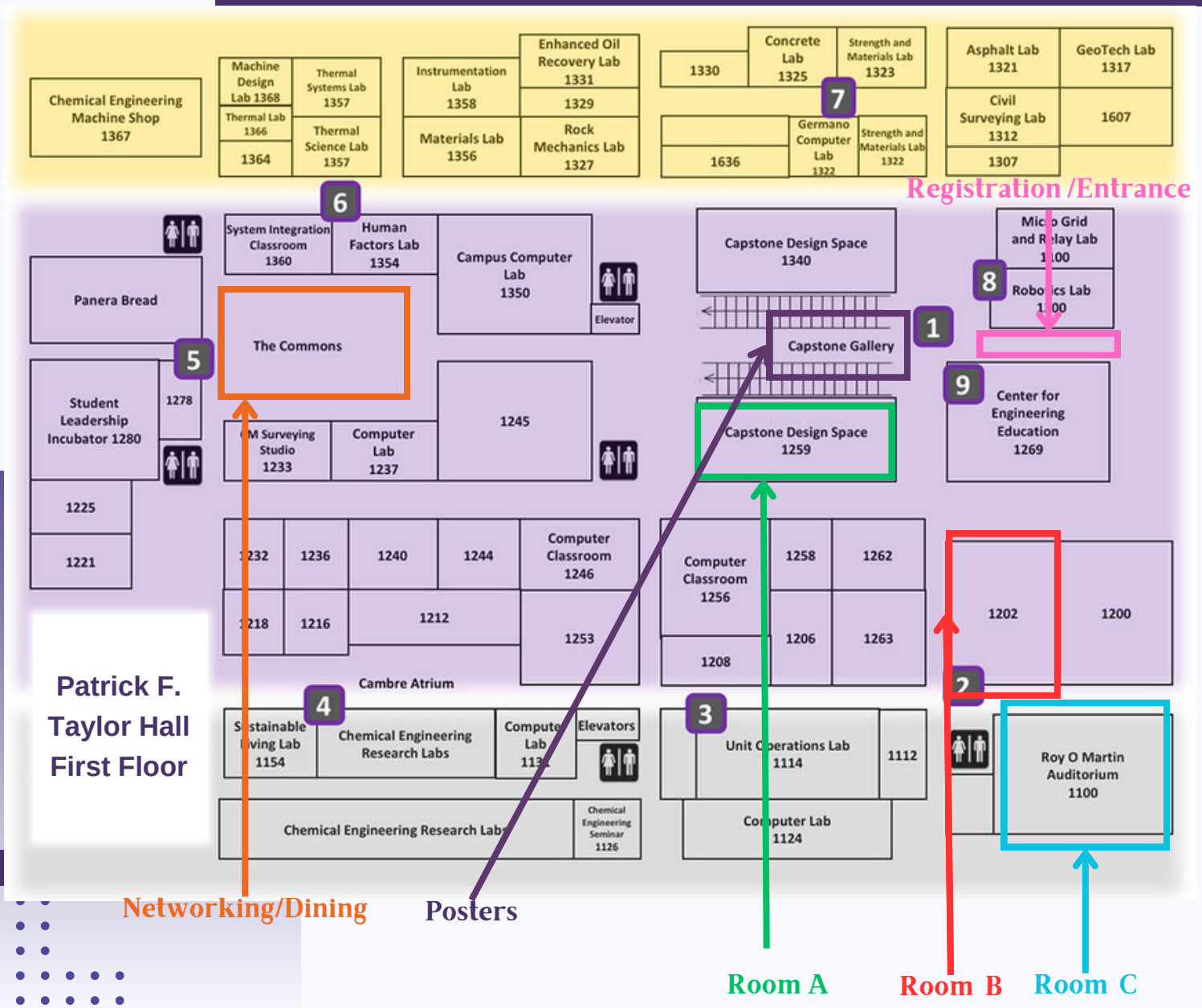

KEYNOTE SPEAKERS

LOCATION: ROOM C (ROY O. MARTIN AUDITORIUM; PFT 1100)

Dr. Elizabeth Kelley

Instrument Scientist:
NIST Neutrons for Research Center

Scattering and squishy science: my adventures in neutron scattering and soft matter

Soft materials play an essential role in our everyday lives, from the cream in our coffee to the molecules that make up our cells. But why are soft materials soft? And how do we measure squishiness? In this talk, I will share my journey from polymer chemist to beamline scientist in search of a better understanding of the macroscopic properties and functions of these materials from a molecular level. I will also highlight some of the useful neutron scattering tools I learned along the way to probe the nanoscale structure and dynamics of soft materials and the unique insights these tools can provide into next generation polymers.

Dr. Ronald Castellano

Professor:
University of Florida

Homochiral Supramolecular Polymers from Cyclophane Monomers

Synthetic supramolecular polymers (SPs) are now rivaling the form and function of biopolymers through advancements in chemical synthesis but also a sophisticated understanding of how monomer structure dictates assembly thermodynamics, kinetics, and expressions of chiral information. In recent years we presented the idea that “covalent fixation” of two self-assembling SP monomers to produce a self-assembling cyclic dimer could lead to unique atomic level control of structure, dynamics, and stereochemistry on the supramolecular level. Our design features hydrogen bonding (H-bonding) between chiral cyclophanes through appropriate functional groups (e.g., amides); the result is a homochiral one-dimensional nanostructure featuring a double helical array of H-bonds, reminiscent of both peptides and DNA. The motif is robust, persisting in solution and the solid state (with little exception) despite changes in bridge structure, H-bonding unit structure/connectivity, and substituents. Structure-property relationships will be discussed showing how the assembly thermodynamics, and self-association energies, can be tuned over several orders of magnitude by small structural changes to the monomers. In hydrocarbon solvents these systems exist as processable supramolecular polymers. More sophisticated monomer designs will be presented that could provide new ways to probe, and even control, supramolecular polymer mechanism.

CAREER DEVELOPMENT: CAREER PANELISTS

APTEC

LOCATION: ROOM C (ROY O. MARTIN AUDITORIUM; PFT 1100)

Dr. Brandon Chan

Patent Attorney: Duane Morris LLP (New York City, NY)

Dr. Anthony Engler

Assistant Professor: Louisiana State University

Dr. Ly Ngo

Chemistry Instructor: Louisiana State University

Dr. Anthony Mai

Research Scientist: Indorama Ventures IOD (Houston, TX)

Dr. Samuel Bynum

Postdoctoral Fellow: U.S. Naval Research Laboratory

CAREER DEVELOPMENT: SPEAKERS

APTEC

LOCATION: ROOM C (ROY O. MARTIN AUDITORIUM; PFT 1100)

Quynh Do

Graduate Student:
Louisiana State University

Key Principles of Visual Communication Design

Scientists communicate visually through their presentations, posters, and figures. Well-designed presentation materials are critical in constructively educating others about specialized topics and introducing new ideas. Good visuals are also essential to relay data and information effectively. A set of guidelines and considerations in line with fundamental graphic design principles will be presented. The tools gained in this presentation will aid in the creation of visuals that can convey data and concepts in an understandable, accessible manner.

Marlo Milton

Recruiter:
Oak Ridge Associated Universities

Resume Workshop: Your Professional Brand

Welcome to our Resume Workshop, where we will go over important details for crafting a professional brand that showcases your unique skills, accomplishments, and potential. We will go over topics to help you create a compelling introduction that makes employers take notice. Marlo Milton brings more than 14 years of high-volume, full-cycle recruitment experience for industries such as healthcare, finance, administration, not-for-profit, and human resources. Marlo is an Army veteran and has a passion for veteran recruitment. She currently recruits for various ORAU opportunities and is passionate about candidate experience. She strives to provide white glove service to her customers and candidates throughout every stage of the recruitment and hiring process.

Oral Presentations: Session I

10:15 AM-11:25 AM

ROOM A

1) Jaylen Davis, University of Southern Mississippi

10:15 AM-10:35 AM

Synthesis and Characterization of Novel Polybenzoxazine Vitrimers

In this work, benzoxazine monomers were synthesized using bio-derived phenolic acids coupled with alcohols to yield ester-containing benzoxazine monomers. The structure of the monomers was confirmed by NMR and FTIR. Thermal stability and cure profiles of the monomers were investigated using TGA, DSC and rheology, revealing cure temperatures as low as 150 °C compared to traditional polybenzoxazine networks. The resulting polybenzoxazine networks showed a range of Tg's, (20-100 °C) highlighting the versatility of the material for specific applications. Due to the inherent tertiary amines of the benzoxazine structure and neighboring ester-alcohol moieties, these materials undergo transesterification reactions driven by internal catalysis. The vitrimeric behavior of the polybenzoxazines was studied by conducting stress-relaxation experiments via DMA, which revealed relaxation times as fast as 6.5s at 170 °C. DMA and TMA were used to evaluate the topology freezing temperature (Tv) of the materials, resulting comparable values across various techniques. The reprocessability of these materials were confirmed via repeated pulverization and melt pressing procedures. DMA and tensile testing of the reprocessed vitrimers confirmed retention of key properties such as Tg, modulus, and yield stress.

2) Hala Farghaly, University of Houston

10:35 AM-10:55 AM

Dielectric properties of waterborne polyelectrolyte grafted nanoparticles films as sustainable energy storage media

The demand for high energy and power density storage devices is driving the advancement of polymer-based dielectric capacitors. Commonly, polymer nanocomposite-based capacitors have relied on harsh solvents for processing, specifically while making film capacitors. However, the need for a sustainable future necessity the use of green processing solvents, such as water. To this end, solution processable polymer grafted dielectric nanomaterials from aqueous media has attractive features to solve this challenging problem. In this study, we design polyelectrolyte grafted Silica nanoparticle based dielectric polymer grafted nanoparticle (PGNP) films, that can be cast from aqueous solution, as novel energy storage media. The polyelectrolyte grafted layer is critical for the aqueous processing of these hybrid nanomaterials. Our dielectric measurements show that the grafting of SiO_2 nanoparticles into PAA enhances the dielectric permittivity over the SiO_2 nanoparticles and decreases the dielectric loss compared to un-grafted PAA to much lower values. Furthermore, it has a positive impact on the dielectric strength value and increases the energy density 3 times compared to Ungrafted PAA at 50 Hz. By increasing temperature above Tg, both un-grafted PAA and grafted samples show thermal stability ensuring consistent dielectric performance across a wide temperature range, making it reliable for operation in demanding environments. To our knowledge, this study is the first report on the dielectric performance of PAA grafted onto SiO_2, and we will present more results on the use of water-based solutions to fine-tune the performance of PAA-functionalized PGNPs.

Oral Presentations: Session I

10:15 AM-11:25 AM
ROOM A

3) Sandhiya Thiagarajan, The University of Alabama

10:55 AM-11:15 AM

Development of Elastic SEBS bead additives to enhance the recovery behavior of Magnetorheological Fluids

Magnetorheological fluids (MRFs) are mixtures of magnetic particles in a non-magnetic liquid. Upon application of a magnetic field, MRFs change from a liquid to a solid-like state due to the formation of chain-like structures inside the liquid arising from the attraction between magnetic particles. MRFs applications include vibrational dampers, magnetic brakes and prosthetics. However, MRFs lack elastic properties that limits the complete recovery behavior of formed chains on removal of the magnetic field. This study developed elastic SEBS (Styrene-Ethylene-Butylene-Styrene) beads for the first-time to address this challenge. SEBS is a thermoplastic polymer studied for its ballistic capabilities, self-healing performances, and footwear applications. SEBS elastomer of different SEBS: mineral oil ratios, known to have varying mechanical properties were prepared first. Then SEBS beads were developed by stabilizing SEBS-Mineral oil elastomer in water using a surfactant. The rheology and microscopy of the resulting SEBS beads was studied as a function of SEBS:Mineral oil weight ratio, SEBS elastomer concentration, and surfactant concentration. Initial results suggest that the surfactant required to create beads is dependent both on SEBS elastomer concentration and SEB:mineral oil ratio. Rheological results suggest that majority of the developed SEBS bead mixtures exhibited shear thinning behavior. Microscopy analysis of the beads show that bead size increase with increasing SEBS-Mineral oil elastomer concentration. Based on the results obtained an in-depth analysis of experimental conditions to develop stable SEBS elastic beads is presented.

Oral Presentations: Session I

10:15 AM-11:45 AM
ROOM B

4) Dr. Steve Rick, University of New Orleans

10:15 AM-10:35 AM

Simulation studies of stimuli responsive polymers

Stimuli-responsive polymers are materials which show large reversible structural changes in response to small changes in the environment. Recent work in our lab has examined the various roles that hydrophobicity, electrostatic interactions, and hydrogen bonding play in the response. Results for pH and thermal responsive polymers will be discussed.

5) Rahul Kumar, Tulane University

10:35 AM-10:55 AM

Chain architecture impacts the stability of vertical lamellae in block copolymer thin films

Block copolymer (BCP) thin films with lamellar nanostructures oriented vertically to the substrate surface are a potential alternative to photolithography for patterning nanoscale features. Previous studies have shown that chain cyclization reduces the BCP feature sizes and improves thin film stability, but the orientation control of the film is also desired for lithography. Here, we use dissipative particle dynamics (DPD) simulations to study the relative stability of vertical (vs. horizontal) lamellae formed by linear and cyclic BCPs. To mimic experiments, BCP chains are confined between a substrate (2D lattice of DPD beads), and a “gas” bath (DPD beads). With non-preferential surface interactions (same interactions for either block with the "gas" and with the substrate), both linear and cyclic BCPs form vertical lamellae as expected. To test the relative stability of vertical lamellae, we increase the substrate surface preference in a series of steps for one of the blocks until the lamellae orient horizontally to the substrate. We find that the vertical lamellae are more stable for linear BCPs than for cyclic BCPs. These findings suggest that the substrate neutrality condition for vertical lamellae is less stringent for linear BCPs than for cyclic BCPs. We explain these differences induced by differences in chain architecture based on near-surface chain orientations and free energy calculations.

Oral Presentations: Session I

10:15 AM-11:45 AM
ROOM B

6) Moustafa Zagho, University of Southern Mississippi

10:55 AM-11:15 AM

Surface Modification of Poly(vinylidene fluoride) Microfiltartion Membranes Using Polydopamine in Combination with Organic or Inorganic Hydrophilic Agent to Improve Oil Fouling Resistance

Membrane technology is widely utilized for producing industrial-grade water for numerous applications. Poly(vinylidene fluoride) (PVDF) is one of the most commonly used polymers in various separation membranes due to its high mechanical strength, low cost, superior thermal stability, and excellent chemical resistance properties. However, PVDF membranes mainly suffer from oil fouling due to their hydrophobic nature. In this regard, a simple surface modification method based on dopamine polymerization to polydopamine (PDA) is applied to enhance the hydrophilicity and oil antifouling behavior of PVDF membranes. PDA makes strong adhesion to organic and inorganic substrates due to the formation of strong covalent and noncovalent bonds in addition to the presence of abundant surface hydrophilic functional groups such as amines and hydroxyl groups. Modification of PDA is recommended to further enhance the hydrophilicity of the membranes. Herein, we investigated a facile approach which is based on a co-addition of PDA with another either organic (BoltornTM fourth (H40) pseudo-generation 2,2-bis(hydroxymethyl)propionic acid based hyperbranched polyol) or inorganic (MXene) hydrophilic agents. Comparisons are drawn between the effects of incorporating BoltornTM H40 hyperbranched polyol and MXene in combination with PDA on the oil separation performance of PVDF membranes while treating oil-in-water emulsions with a detailed surface characterization of the modified membranes. The incorporation of H40 hyperbranched polyol demonstrated a remarkable boost in the separation of oil from water in tight emulsions while displaying high resistance to fouling over multiple runs versus unmodified, PDA, and PDA/MXene modified PVDF membranes. The reported functionalized microfiltration membranes, especially the PDA/H40/PVDF membrane, can be recommended for water/oil separations.

7) Micheal Dearman, Louisiana State University

11:15 AM-11:35 AM

Versatile strategies to tailor the glass transition temperatures of bottlebrush polymers

This talk presents a strategy for tailoring the glass transition temperatures of bottlebrush polymers by manipulating various parameters, such as side chain length, backbone length, molecular weight composition, and topology. The study explores the impact of these parameters on the glass transition behavior of bottlebrush polymers and demonstrates a wide range of Tg values can be accessed through side chain engineering. The precision bottlebrush polymers (PBPs) used in the study yield precise Tg values, some of which can only be achieved through blending at the cost of Tg broadening. Additionally, multiblock PBPs offer the ability to target arbitrary Tg values while maintaining a sharp glass transition, combining the advantages of both approaches. Overall, the findings highlight the versatility of side chain engineering strategies in controlling the glass transition behavior of bottlebrush polymers.

Oral Presentations: Session I

10:15 AM-11:45 AM
ROOM C

8) Catherine Sarantes, University of Southern Mississippi

10:15 AM-10:35 AM

Blocked Isocyanates for Covalent Adaptable Polyurethanes: Chain Extension

Polyurethanes and polyureas (PUs) are versatile polymeric materials widely used in various industrial applications but suffer challenges in reuse and recycling. Recent efforts to address these challenges include the exploitation of the dynamic nature of the urethane/urea bonds to enable materials reprocessing. In this presentation, we explore the synthesis and use of imidazole-terminated chain extenders as dynamic building blocks for PU thermosets. Many approaches were taken to access liquid imidazole diamine monomers including Sn2 etherification, glycidyl etherification, silylations, Fisher esterifications, Steglich esterifications, and amidations, but synthetic roadblocks were met at the chain extender creation and imidazole attachment stages. Chain extenders were prepared via etherification of bisepoxides with 1H-imidazole-5-methanol. Increasing the molecular weight between the terminal imidazole functional groups with aliphatic components enabled creation of low viscosity liquid and wax-like building blocks that are readily miscible with isocyanates for network formation. This approach eliminated the need for additional additives such as plasticizers simplifying the system to a formulation akin to a traditional 2K polyurea. Ultimately, we explored the progression of several approaches for diol chain extension and installation of the imidazole functionality followed by the development of a safer and easier method to process library of chain extended aliphatic diamines.

9) Mina Shanbedi, University of Houston

10:35 AM-10:55 AM

Introducing 3D structure combined nanofillers to gel polymer electrolytes for enhancing energy storage and thermal fluctuation durance

Halloysite nanotubes (HNTs) have been used as an effective electrolyte additive for the first time and were aligned in the Z direction by the assistance of high voltage electric field, which helps building direct paths for the ions to transfer through channels with ultra-high ionic conductivity because they are filled with ionic liquid (IL). Comprehensive electrochemical properties along with thermal properties of these SCs will be closely scrutinized in this work. As another approach to enhance the the storage performance of the supercapacitor another less studied nanofiller, hexagonal boron nitride, was introduced to the current work and magnified the energy storage and capacitance of the system.The incorporation of h-BN nanosheets into the PVA-H2SO4 gel polymer, serving as both electrolyte and separator, results in a quasi-solid-state supercapacitor exhibiting notable characteristics, including elevated specific capacitance, commendable rate capability, and exceptional cycle stability. Operating at a current density of 0.5 A g-1, the quasi-solid-state supercapacitor achieves an electrode-specific capacitance of 133.5 F g-1, retaining an impressive 96.78% capacitance even after undergoing 2000 charge-discharge cycles. This h-BN nanosheets-doped Gel Polymer Electrolyte (GPE), marked by its excellent performance and straightforward synthesis methodology, emerges as a promising contender for high-performance quasi-solid-state supercapacitors and various electrochemical devices encompassing rechargeable batteries and fuel cells. Furthermore, this study illuminates the potential use of 2D materials in advanced Gel Polymer Electrolytes (GPEs).

Oral Presentations: Session I

10:15 AM-11:45 AM

ROOM C

10) Elizabeth Bury, University of Alabama

10:55 AM-11:15 AM

Mechanical Impact of Paraffinic Oil on the Thermoplastic Triblock Copolymer Styrene-Ethylene-Butylene-Styrene

The majority of deformable electronics and sensors rely on soft polymeric materials as the continuous phase to either encase components or act as the matrix for composites in order to increase conformability and biocompatibility at the human-machine interface. Extensive research has been performed utilizing thermoset polymers, such as polydimethylsiloxane (PDMS), for deformable electronic applications. However, thermoset polymers have many limitations when utilizing them as the continuous polymeric material, including an intensive and lengthy fabrication process at both the lab-scale and industrial-scale. Thermoplastic polymers, however, are significantly easier to process as they have the intrinsic ability to be re-molded at temperatures above their melting point and re-solidified into different desirable configurations upon cooling, thus allowing for polymeric materials that are adaptable, cost-effective, and tailorable. In this work, the mechanical behavior of the thermoplastic triblock copolymer styrene-ethylene-butylene-styrene (SEBS) has been investigated at different concentrations of the SEBS solid swollen in paraffinic oil to result in tailorable bulk polymer modulus and elasticity. The rigidity, elasticity, and melting behavior of the SEBS was found to be tunable through paraffinic oil selection. The mechanical behavior and fabrication parameters of host polymeric materials are vital factors for selecting the best polymer for specific deformable electronic and sensor applications. Fundamental mechanical characterizations, such as this, will enable future work to be further informed about the importance that the relationship and impact of utilizing specific polymers and their formulations have on deformable electronics and sensors.

11) Samantha Daymon, University of Southern Mississippi

11:15 AM-11:35 AM

Molecular dynamics simulations of shockwave propagation in amorphous polyisobutylene (PIB) system

The development of polymer structures with improved shockwave resistance is an area of growing interest. Experimental measurements of shockwave characteristics are difficult to perform due to the extreme pressures, and temperatures, as well as the very short timescale of the shockwave responses. However, molecular dynamics (MD) simulations are easily able to track molecular movements within polymer systems under extreme conditions at picosecond timescales, thus allowing for a fundamental study of shockwave behavior. This work investigated the shockwave behavior in polyisobutylene (PIB), a rubbery polymer renowned for its high damping capacity. We simulated the shockwave response in PIB using two shock methods, non-equilibrium molecular dynamics (NEMD), and multi-scale shock technique (MSST). Throughout these simulations, we tracked the evolution of kinetic parameters, as well as bulk quantities such as average speed, density, and pressure. NEMD is a more computationally expensive method, but it provides more information about shock response including a profile shape. A comparison of piston and shock velocity for both methods show a deviation at lower piston velocities but convergence at high velocities. This difference was attributed to the progression of the shockwave shape profile from a broad transition at low velocities to narrow (almost instantaneous) transition at high piston velocities.

Oral Presentations: Session II

1:00 PM-2:30 PM
ROOM A

12) Chamberlain Amofa, Louisiana State University

1:00 PM-1:20 PM

Tailoring Janus Nanoparticle Surface Chemistry with Polymer Ligands

Polymer-coated Janus nanoparticles (NPs) remain a complex system with inherent heterogeneity in both surface and core size. Despite efforts to control polymer dispersity, achieving absolute uniformity remains a major challenge. To address this challenge, we synthesized linear polymers from four main monomer families: styrene, dimethyl siloxane, tert- butyl acrylate, and methyl acrylate. Importantly, the structural parameters of these ligands—chain length, dispersity, and chemical immiscibility control the behavior of NP. It is anticipated that NPs with precise surface chemistry will pave the way to integrate an organic shell with tailored functionalities and an inorganic core.

13) John Konlan, Louisiana State University

1:20 PM-1:40 PM

Development of a Multifunctional Self-Healing Composite Laminate with Shape Memory Alloy Z-Pins

Laminated composites with multifunctionality are highly desired in modern lightweight engineering structures. The purpose of this study is to develop a robust-lightweight self-healing multifunctional composite laminate with delamination healing, impact tolerance, strain sensing, joule heating, deicing, and room temperature shape restoration functionalities. In this study, a novel self-healable and recyclable vitrimer-based shape memory polymer (VSMP) was used as the matrix, unidirectional Saertex glass fabric was used as reinforcement, and tension programmed shape memory alloy (SMA) wires (Flexinol) were used as z-pins. This design followed the strategy of close-then-heal (CTH) for delamination healing. The goal of the sinusoidal z-pins is to facilitate the narrowing of delamination opening by the CTH strategy, making it possible for the vitrimer to complete the healing of the laminate. To provide multifunctionality, the programmed SMA wires were further twisted and formed into sinusoidal shape. Copper wire strands were hooked to the sinusoidal SMA z-pins to make the SMA z-pins a closed circuit. Low velocity impact (LVI), compression after impact (CAI), self-healing of impact induced delamination, deicing, and room temperature shape restoration tests were conducted. The tests result show that the desired multifunctionality of the laminated composite was achieved. The novel hybrid composite laminate provides a promising sustainable multifunctional material system for lightweight load-carrying engineering structures.

Oral Presentations: Session II

1:00 PM-2:30 PM
ROOM A

14) Anwar Shafe, Louisiana Tech University

1:40 PM-2:00 PM

Identification and Design of Better Diamine Hardened Epoxy Based Thermoset Shape Memory Polymers: Simulation and Machine Learning

Shape memory polymers (SMPs) can temporarily deform and then return to their original shape upon exposure to an external stimulus, making them attractive for various applications. Nevertheless, current SMPs often face limitations in recovery stress. This study tackles these limitations by employing molecular dynamics and machine learning to identify novel amine-hardened, diglycidyl-ether-based epoxy systems with enhanced shape memory properties. We calculated atomistic and topological fingerprints for a training dataset. These fingerprints were then used to train machine learning algorithms to predict stress recovery. Subsequently, machine learning algorithms were employed to identify the most promising candidates from a large pool of semi-automated candidates. These candidates underwent further evaluation through atomistic molecular dynamics, leading to the identification of several excellent SMP candidates with superior stress recovery capabilities.

15) Dr. Jimmy Lawerence, Louisiana State University

2:00 PM-2:20 PM

Chemically Versatile & Scalable Strategies to Prepare Precision Branch Polymers

Over the past few years our group has developed a highly efficient synthesis-separation based strategy to design topologically precise and discrete bottlebrush polymers. Beyond enabling new strategies to tailor glass transition temperatures, this talk will also describe how the same strategy can be used to create diverse new materials with properties precisely and solely defined by side chain physics.

Oral Presentations: Session II

1:00 PM-2:30 PM

ROOM B

16) Shanta Biswas , Louisiana State University

1:00 PM-1:20 PM

Effects of Molecular and Macromolecular Crowding Agents on Protein/Polymer Complex Coacervation

Complex coacervation refers to the liquid-liquid phase separation (LLPS) due to the strong associative interactions between charged macromolecules. In recent years, the study of complex coacervation has been used to explain the formation of biologically important membraneless organelles (MLOs). MLOs are believed to be formed by the LLPS between protein and nucleic acid within the living cellular environment. However, the impacts of the crowded intracellular environment on the behavior and interactions of biomolecules involved in MLOs formation are not fully understood. In this context, we aim to investigate the effects of crowding on a model protein/polymer complex coacervate system. To introduce such crowdedness into our model system, sucrose and polyethylene glycol (PEG) have been used as molecular and macromolecular crowders, respectively. Our findings demonstrated that bigger coacervate droplets, increased protein/ polymer content, and higher density of the coacervate phase were observed in PEG as compared to the coacervate prepared in sucrose. These differences in coacervate properties can be attributed to the effects of crowders on individual macromolecules, such as the conformation of model polymers and non-specific interactions among model protein molecules. Furthermore, our findings show that sucrose gets distributed in both the coacervate and dilute phases, whereas PEG is excluded into the dilute phase only. Collectively, our findings shed light on understanding the effects of crowding on complex coacervation while highlighting the formation and properties of coacervates in the context of MLOs.

17) Ruchi Patel, Louisiana State University

1:20 PM-1:40 PM

pH-dependent interfacial activity of perfluoroalkyl carboxylic acids (PFCAs)

The ubiquity of perfluoroalkyl carboxylic acids (PFCAs) in both atmospheric and environmental water is well-documented. Nonetheless, huge discrepancies exist in the reported pKa values for PFCAs, often spanning three to four units. These disparities stem from an incomplete understanding of how pH influences the ionized state of PFCA molecules in bulk solution and at the air-water interface. Using pH titration and surface tension measurements, we show that the pKa of the PFCA adsorbed at the air-water interface differs from the bulk. We systematically explore how the length of the fluoroalkyl tail of PFCAs influences their surface-pKa and interfacial activity across a broad pH range. Our study reveals a crucial consequence of PFCA accumulation at the air-water interface: a reduction in the evaporation rate of microdroplets, which would further impact the stability of atmospheric aqueous aerosols containing PFCAs. This study underscores the potential significance of pH in directing the dynamics of atmospheric aerosol droplets containing PFCAs and prompts the inclusion of pH as a key determinant in the predictions of their fate.

Oral Presentations: Session II

1:00 PM-2:30 PM
ROOM B

16) Dr. Meng Zhang, Louisiana State University

1:40 PM-2:00 PM

Understanding the Role of Charge Patterning on the Solution Structure of Polypeptoid Multi-block Copolymers (mBCPs)

Ionic amphiphilic block copolymers (ABCs) consist of a hydrophilic segment and a hydrophobic segment with the placement of ionic groups, and they can self-assemble into core-shell type structures in selective solvents. The micellization of ionic ABCs can be influenced by various driving forces, including electrostatic interactions, crystallization interactions, and hydrophobic interactions. Early studies have shown that ionizable groups randomly distributed along the polymer sequence can effectively modulate the solution micellar structure, while the role of charge pattern is still in its early stages. Polypeptoids are a category of structural mimics of polypeptides with an N-substituted polyglycine backbone. Due to N-substitution, polypeptoids are unlikely to form a secondary structure and are free of hydrogen bonding interactions, making them an ideal system to study the electrostatic interactions encoded in the polymer sequence. In this work, we have synthesized three ionic polypeptoid block copolymers with one ionizable group placed either at the hydrophilic segment terminus, the junction of the hydrophilic and hydrophobic segments, or randomly distributed along the hydrophilic segment, while another ionizable group was fixed at the hydrophobic segment. These ionic polypeptoid block copolymers self-assembled into a core-shell ellipsoidal structure, and the aggregation structure was tuned by the solution pH and ionizable group position.

17) Jason Wiley, Louisiana Tech University

2:00 PM-2:20 PM

Control of Particle-particle and Lamellar Spacing in Lamellae-forming Block Copolymer Grafted Nanoparticles by MD Simulation Using Protracted Colored Noise Dynamics (PCND)

Enhanced materials are critical enables across various industries, with advancements in properties showcased in diverse materials, particularly nanoparticle-polymer composites, through hierarchical structures and assemblies. While previous studies have demonstrated the dispersion and coarse placement of particles within the polymer matrix using Janus particles or homopolymer grafts, achieving precise control over particle placement remains challenging. This research focuses on the potential of block copolymer grafted nanoparticles to provide fine control over nanoparticle placement, employing coarse-grained molecular dynamic (MD) simulation coupled with protracted colored noise dynamics (PCND). The study demonstrates that lamellae-forming block copolymers grafted onto spherical nanoparticles exhibit hexagonal packing at sufficient graft density, allowing for meticulous control over both particle-particle and lamellar spacing.

Oral Presentations: Session II

1:00 PM-2:30 PM
ROOM C

18) Wencai Li, Louisiana State University

1:00 PM-1:20 PM

Structural health monitoring of ultrasonically welded thermoplastic composite joints using embedded multifunctional films

Thermoplastic composites (TPCs) are becoming more prevalent, particularly in large or integrated structural components, necessitating effective joining techniques. Fusion bonding, specifically ultrasonic welding (USW), has emerged as a promising method for TPCs, leveraging their capacity to be reshaped through heating and cooling. This eliminates the need for mechanical fasteners or reduces curing times and minimizes surface preparation. USW, with its rapid cycling time and potential for automating assembly of large-scale structures, holds promise for substantial energy consumption reduction. However, the limited industrial applications of USW underscore the need for deeper insights into the process to instill confidence in its utilization. Moreover, the susceptibility of composite structures to damage requires structural health monitoring (SHM) during their service life. This study focuses on SHM of TPC joints using embedded multifunctional films at the bond line. The research explores the films' influence on the USW process for TPC joints and assesses their impact on mechanical performance. The addition of multi-walled carbon nanotubes (MWCNTs) at 15 and 20 wt% demonstrated negligible effects on the welding process. However, at 25 wt%, a 39% reduction in lap shear strength (LSS) occurred due to increased brittleness. Subsequently, welded joints with nanocomposite films containing optimized MWCNT concentrations (15 wt%) exhibited potential for damage monitoring. This was achieved through real-time electrical resistance changes at the weld interface under tension, periodic bending, and monotonic/cyclic flexural loading. These findings contribute valuable insights for the application of USW in TPC structures, addressing both the welding process and damage monitoring.

19) Philip Brahana, Louisiana State University

1:20 PM-1:40 PM

Photooxidation of micro plastics

Microplastics are ubiquitous in the environment, leading to a new form of plastic pollution crisis, which has reached an alarming level worldwide. Micron and nanoscale plastics may get integrated into ecological cycles with detrimental effects on various ecosystems. Commodity plastics are widely considered to be chemically inert, and alterations in their surface properties due to environmental weathering are often overlooked. This lack of knowledge on the dynamic changes in the surface chemistry and properties of (micro)plastics has impeded their life-cycle analysis and prediction of their fate in the environment. Through simulated weathering experiments, we delineate the role of sunlight in modifying the physicochemical properties of microplastics. Within 10 days of accelerated weathering, we observe that an altered physiochemical state of microplastic pollutants affects their dispersibility in water, pollutant uptake capacity and ice nucleation ability.

Oral Presentations: Session II

1:00 PM-2:30 PM
ROOM C

20) Nduka Ogbonna, Louisiana State University

1:40 PM-2:00 PM

Designing Precision Bottlebrush Polymers with Tailored Side Chains for Enhanced Solubilization and Improved NMR Dynamics

Water-soluble fluorinated MRI contrast agents are safer alternatives to metal-based platforms for disease diagnosis; however, improving the fluorine signal comes with the cost of aqueous solubility. This talk will discuss the synthesis of a new fluorine-rich bottlebrush polymer with high solubility in biological media. Key to this synthetic approach is the design of the hydrophilic side chains' sequence, composition, and dispersity. The impact of structural design on NMR dynamics will be discussed. Overall, we aim to show the sequence for optimal performance, offering a safe and promising disease diagnosis and therapy solution.

21) Kennedy Guillot, Louisiana State University

2:00 PM-2:20 PM

Synthesis of rough patchy colloids through selective polymer swelling

Developing new methodologies to engineer anisotropies in microscopic particles has become a well-researched topic in colloid science. Anisotropic properties of particles can influence their phase behavior, mimicking structures originally exclusive to nature or even assembling into novel structural motifs. Several mechanisms have been utilized over the years to fabricate anisotropic particles, including manipulating a "patch" on the particle surface to promote surface heterogeneity. However, current fabrication techniques often produce patches that contain chemical and physical anisotropies, making it difficult to identify the driving force behind self-assembly. To overcome this challenge, we produced a new approach to synthesize these microscopic particles with well-defined rough patches on the surface. We used non-crosslinked polystyrene (PS) treated with vapors of a good solvent, here an acetone-water mixture, to achieve surface patches that are chemically similar yet also physically rough. Rough patch formation is governed by the selective condensation by the acetone-water vapors on the apex of the polystyrene microparticle surface, which is consistent with Volmer's classical nucleation theory. Polymer surface corrugation can be precisely tuned through the manipulation of the vapor-liquid equilibrium of the volatile acetone mixture, with the dependence of patch formation based on particle and substrate wettability. Condensation of the vapor will only occur on the particle surface when it is more wettable than the substrate. This presentation will highlight the mechanism of formation of these roughness-controlled patchy particles through experimental and molecular dynamics simulations to identify the role of the rough patches on self-assembly behavior.

Poster Presentations

2:15 PM-3:15 PM
CAPSTONE GALLERY, PATRICK F. TAYLOR

1 Mahi Ahmad

Institution: Tulane University
Title: Cyclization of Linear Ethylene Brassylate

2 Amman Nadeem

Institution: Tulane University
Title: Synthesis of Linear and Cyclic Poly(hydroxypivalic acid)

3 Brennan Curole

Institution: Tulane University
Title: Dithiol-yne based Poly-hydroxy Dendrimers for High Dielectrics Constants

4 Erin Tsai

Institution: Louisiana State University
Title: Modulation of the Self-Assembly Dynamics of Binary Mixtures of Ionic, Sequence-Defined Polypeptoid Oligomers in Aqueous Solution

5 Robert Herman

Institution: Louisiana State University
Title: Ring-Opening Alkyne Metathesis Polymerization of Conjugated, Strained Nanohoops

6 Dominic Adrewie

Institution: Louisiana State University
Title: Preparation of thiol-ene gel systems for frontal Polymerization

7 Fahima Shaon

Institution: Louisiana State University
Title: Formation and Characterization of Temporal Controlled Thermoset Adhesive Based on Thiol-Michael Addition Triggered by Urea-urease Clock Reaction using Watermelon Seed Powder (WMSP)

8 Kingsley Yeah Gayabaah

Institution: Southern University and Agricultural and Mechanical College
Title: High Performing Shape Memory Regolith Composite Material for Extra-Terrestrial Application

Poster Presentations

2:15 PM-3:15 PM
CAPSTONE GALLERY, PATRICK F. TAYLOR

9 Dr. Yahua Sun

Institution: Southeastern University
Title: Multifunctional carbon nanotubes-glass fiber-epoxy composites with high microwave absorption

10 Harry Spencer

Institution: Louisiana State University
Title: Effects of electron withdrawing and donating substituents on the mechanochemical cleavage rate of a phenyl ester mechanophore

11 Georniphа Milbin

Institution: Louisiana State University
Title: Molecularly Imprinting Benzyl Fentanyl for the Detection of Fentanyl

12 Trey Schneider

Institution: University of Southern Mississippi
Title: Covalently Incorporating Ceramics into High-Char Yielding Polymers

13 David Walker

Institution: University of Southern Mississippi
Title: Modifying Bismaleimide Monomers with Nitrile Functionalities

14 Stefani Klisch

Institution: Louisiana State University
Title: Rotation of Light Activated Molecular Motors in a Polymersome Environment

15 Md Abdullah Al Mahmud

Institution: Louisiana State University
Title: A new approach to cure-on demand coatings using with ammonia to catalyze thiol-epoxy and thiol-acrylate reactions.

16 Tianyi Wang

Institution: Louisiana State University
Title: Graph neural networks for predicting the thermodynamic and dynamics properties of polymer

Poster Presentations

2:15 PM-3:15 PM
CAPSTONE GALLERY, PATRICK F. TAYLOR

17 Elizabeth Bury

Institution: The University of Alabama
Title: Galinstan Multi-Material Dielectric Polymer Composites for Deformable, Multimodal Capacitive Pressure Sensing

18 Pedram Azizi-Hariri

Institution: Tulane University
Title: The use of amphiphilic polypeptoids to solubilize hydrophobic drugs in peptoid-lipid complexes

19 Bradley Lamb

Institution: University of Southern Mississippi
Title: Investigation of Polyfluoroalkyl substances self-assembly behavior with molecular dynamics simulations

20 Titilayo Oluwole

Institution: Louisiana State University
Title: Topologically Precise Bottlebrush Polymer Surfactant: Synthesis and Characterization.

21 Nicholas Enos

Institution: University of Southern Mississippi
Title: Carbon Fiber Influence on Poly (ether ketone ketone) Crystallization Kinetics and Morphology

22 Abubakar Sumaila

Institution: Southern University and A&M College
Title: Investigation of Thermal and Mechanical Properties of Hybrid Activated Sugarcane Bagasse Reinforced Laminate Composites

23 Emmanuel Aidoo

Institution: Southern University and A&M College
Title: Characterizing Low-Velocity Impact Response of Composite Laminates Reinforced with Agricultural Waste Fillers

24 Anusha Vonteddu

Institution: University of Houston
Title: Dynamics of Polyelectrolyte Coacervate Droplets Under External Electric Field

Poster Presentations

2:15 PM-3:15 PM
CAPSTONE GALLERY, PATRICK F. TAYLOR

25 Xiaoshen Bai

Institution: Louisiana State University
Title: Solvent-Free Depolymerization of Plastic Waste Enabled by Plastic-Catalyst Interfacial Engineering

26 Khaleda Chowdhury Rinee

Institution: Louisiana State University
Title: Understanding the Impacts of Nanoparticle Morphology on the Porosity within Aluminum Adjuvant Aggregates

27 Borui Wang

Institution: Tulane University
Title: Facile synthesis of hierarchical mesoporous materials as support of amine-containing polymers for carbon capture

28 Drew Poche, Brad Wurm, Uzam Sha

Institution: Sekisui Industries
Title: Biomass Modified Polyvinyl Alcohol for Practical Applicaitons

29 Anuja Thapa

Institution: Louisiana State University
Title: Synthesis and characterization of polypeptide and polypeptoid polyelectrolyte complexes to understand the effect of molecular characteristics on coacervation

30 Samuel Osowo

Institution: Louisiana State University
Title: Exploring the foldcat hypothesis: Investigating the growth and sequence differentiation of prebiotic polymers through Polypeptoid HP copolymers

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