Georgia Tech Renewable Bioproducts Institute

Renewable Bioproducts:
Advances in Lignocellulosics Processes and Products

POSTER SESSION

October 1, 2014

Georgia Tech Hotel and Conference Center

Salons IV-V

[Exit meeting room/turn right/through double-doors—Salons IV-V on right]

Instructions for Poster Judging

- Each guest will receive three tokens.
- Please visit many posters during the poster session.
- Pick your three favorite posters considering the quality of the work, the visual presentation on the poster, and the way the presenter explains the poster (including his/her ability to answer questions).
- Give a token to the presenters of your three favorite posters. Please do not give more than one token to the same presenter.
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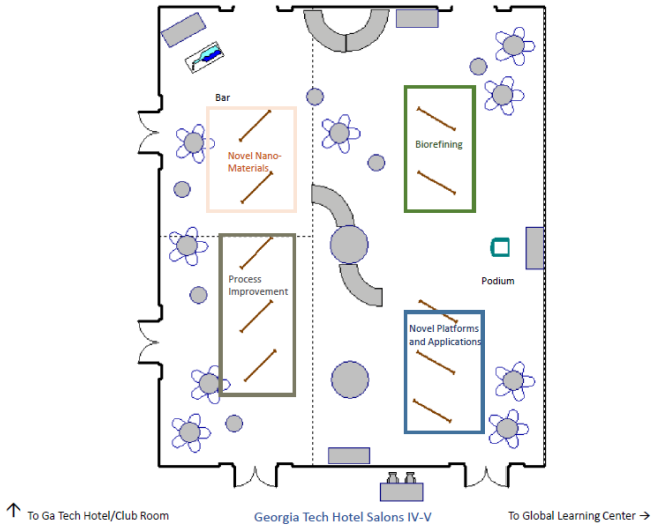

Renewable Bioproducts:
Advances in Lignocellulosics Processes and Products

POSTER SESSION
Oct 1, 2014

Biorefining

	Name	Title	Abstract	Advisor/Schools	Authors
1.	Ewbank, Jessica	Catalytic Conditioning of Biomass Derived Syngas	Gasification of biomass offers the potential to produce syngas from a renewable resource. However, biomass-derived syngas contains significant quantities of methane, carbon dioxide, and tars (condensable aromatics), which need to be reformed to increase the efficiency of the process and to avoid fouling of downstream equipment. Nickel and cobalt catalysts supported on γ-Al2O3 have been shown to be active for the desired reforming reactions. In most reforming studies, impregnation methods are the primary synthesis technique. However, impregnation methods often lead to poor dispersion and catalysts that are prone to sintering and coking under typical reforming conditions. To prepare reproducible and stable catalysts, we utilized controlled adsorption of ionic metal precursors on the support. In this approach, the pH of the impregnating mixture is adjusted to maximize metal support interactions. We find that electrostatic and specific interactions are involved in the adsorption of the metal precursors on the support surface. Physicochemical characterization of the catalysts showed that controlled adsorption results in enhanced metal-support interactions and smaller metal particles compared to catalysts synthesized by impregnation. Reactivity studies for dry reforming of methane illustrated that these properties are responsible for increased conversion and longevity of the catalysts.	Sievers, Carsten Chemical and Biomolecular Engineering	

Biorefining

	Name	Title	Abstract	Advisor/Schools	Authors
2.	Foo, Guo Shiou	Synergistic Effect between Defect Sites and Functional Groups in the Hydrolysis of Cellulose using Activated Carbon	The chemical oxidation of activated carbon by hydrogen peroxide and sulfuric acid is investigated, structural and chemical modifications are characterized, and the materials are used as catalysts for the hydrolysis for cellulose. Treatment with hydrogen peroxide enlarges the pore size while imparting functional groups such as phenols, lactones and carboxylic acids. Sulfuric acid treatment primarily targets the edges of carbon sheets, and this effect is more pronounced with higher temperature. Adsorption isotherms demonstrate that the adsorption of oligomers on functionalized carbon is dominated by van der Waals forces. The chemically treated materials are active for the hydrolysis of cellulose despite the relative weakness of most of their acid sites. It is shown that a synergistic effect between defect sites and functional groups enhances the activity by inducing a conformational change in the glucan chains when adsorbed on defect sites. The exposed glycosidic bonds interact with in-plane functional groups.	Sievers, Carsten Chemical and Biomolecular Engineering	
3.	Kang, Yuzhi	An effective chemical pretreatment method for lignocellulosic biomass with substituted imidazoles	Lignocellulosic biomass is the most abundant, naturally renewable, organic resource for biofuel production. Due to its recalcitrance to enzymatic degradation, pretreatment is a crucial step prior to hydrolysis of the feedstock. A variety of pretreatment methods have been developed and intensively studied to achieve optimal yield without imposing significant adverse impact on the environment. In this work, we present a novel chemical pretreatment method for the first time using substituted heterocycles with ambient conditions in a time-efficient manner. Significant hydrolysis yield enhancement for the subsequent enzymatic process was observed for both cellulose and lignocellulosic biomass. The newly developed chemical pretreatment technique can be potentially utilized in larger scale by itself or in combination with other pretreatment techniques to quickly and effectively reduce biomass recalcitrance for biofuel applications.	Bommarius, Andreas S Chemical and Biomolecular Engineering	Yuzhi Kang, Minjeong Sohn, Jay H. Lee, Matthew J. Realff, Andreas S. Bommarius

Biorefining

	Name	Title	Abstract	Advisor/Schools	Authors
4.	Liu, Hsiang-Hao (Clive)	CNT Incorporated Lignin/PAN Composite Carbon Fibers	As the byproduct of the pulp and biorefinery industry and the second most abundant biomacromolecules on earth, lignin is an attractive cost-effective alternative for carbon fiber precursor. However, the lignin-derived carbon fibers have relatively low mechanical properties. In this work, the authors propose a novel precursor polyacrylonitrile (PAN)/Hardwood Lignin/Carbon nanotubes (CNT) system to balance production cost and carbon fiber mechanical properties. The incorporation of lignin will reduce cost and environmental impact from manufacturing, and the addition of CNT will improve the performance of carbon fibers. Historically, PAN fiber is mostly manufactured via solution-spinning, and lignin fiber is mainly processed through melt-spinning. The authors in this work are utilizing solution-spinning for the composite fibers. Composite fibers are then stabilized under oxidative conditions and further carbonized under inert environment at different temperatures. The structure, processing and properties of these fibers will be presented.	Kumar, Satish Materials Science and Engineering	Clive Liu, An - Ting Chien, Brad Newcomb, Yaodong Liu and Satish Kumar
5.	Mu, Wei	Catalytic hydro-cracking of pyrolysis oil derived from lignin	Aqueous-phase hydrodeoxygenation of lignin pyrolysis oil and related model compounds were investigated using four noble metals supported on activated carbon. Using neutral supporting material and aqueous phase (pH=7) is able to reveal the genuine catalytic behavior of the noble metals. The hydrodeoxygenation of guaiacol has three major reaction pathways. The demethylation reaction, mainly catalyzed by Pd, Pt and Rh, produces catechol as product. The presence of catechol and guaiacol in the reaction is responsible for the coke formation and the catalysts deactivation. As expected, there was a significant decrease in the specific surface area of Pd, Pt and Rh catalysts. In contrast, no catechol was produced from guaiacol when Ru was used, and completely hydrogenation was accomplished. The lignin pyrolysis oil upgrading with Pt and Ru catalysts further validate the reaction mechanism deduced from model compounds. Fully hydrogenated bio-oil was produced with Ru catalyst.	Deng, Yulin Chemical and Biomolecular Engineering	

Biorefining

	Name	Title	Abstract	Advisor/Schools	Authors
6.	Newalkar, Gautami M	The role of process variables in gasification of biomass	High-pressure biomass gasification is poorly understood at heating rates of practical significance. This work addresses this knowledge gap by performing pyrolysis of pine at high temperatures (600–1000 °C) and high pressures (5–20 bar) in an entrained-flow reactor. Heating rates of 103–104 °C/s are achieved with solids residence time ranging from 4 to 28 s. Pyrolysis pressure, temperature, heating rate, and residence time dramatically influence the physical and chemical properties of char, mainly through differences in the release of volatiles, evolution of char morphology, and carbonization of the char skeleton. The surface area and pore properties of chars correlate with the development of graphite-like structures in the carbon matrix. The formation of polynuclear aromatic tars at the longest residence times appears to occur via gas-phase molecular weight growth reactions. Gasification reactivity of chars was measured using 100 % CO_2 or 10% H_2O. Highest temperature and intermediate pressure chars were found to be least reactive. The hydrogen and oxygen functionalities in chars were found to be the best descriptors of gasification reactivity. The catalytic effect of inorganics on cellulose char was found to be in the order: K>Ca>Mg.	Agrawal, Pradeep Chemical and Biomolecular Engineering	Gautami Newalkar, Kristiina Iisa, Carsten Sievers, Pradeep Agrawal

Biorefining

	Name	Title	Abstract	Advisor/Schools	Authors
7.	So, Jungseob	In-situ ATR IR Study on the Mechanism of Aqueous Phase Reforming of Polyols and Sugars	Hydrogen can be produced by aqueous-phase reforming (APR) of biomass-derived polyols and sugars over metal catalysts, such as γ-alumina-supported platinum or tin-promoted Raney-nickel.1-2 The reaction occurs under relatively mild conditions (500K). Side reactions can lead to the formation of alkanes. Early studies presented APR as a new way to convert biomass-derived oxygenates to H_2 for use in fuel cells and also suggested a reaction mechanism, in which C-C cleavage of oxygenated hydrocarbons is followed by the formation CO and H_2. Then, CO is further reacted with water to CO_2 and H_2 by water-gas shift reaction. The exact identification of surface species and their rates of formation and conversion will be required to optimize the reaction activity and selectivity to the side reactions. In our study, *in situ* attenuated total reflectance infrared (ATR-IR) spectroscopy is carried out to investigate APR reactions of polyols and sugars on Pt/γ-Al2O3. With this approach, surface species on a catalyst can be probed effectively while keeping the contribution from the liquid solvent marginal to preserve many important regions of IR spectrum. A sequential pretreatment of degassed H_2O, O_2-saturated H_2O, and H_2-saturated H_2O is demonstrated to be most effective for cleaning 5 wt% Pt/γ-Al2O3 prior to *in-situ* studies on the APR reaction of glycerol, sorbitol, and glucose. As a first step of APR, oxygenated hydrocarbons are converted into CO in bridging and linearly bound coordination on the surface of the Pt particles. The CO species on bridging sites are converted significantly faster by the water-gas shift (WGS) reaction to produce CO_2. Kinetic studies on the conversion of different oxygenates are conducted to extract semi-quantitative parameters to compare the rate of reactions. In particular, it is shown that the size of the oxygenate molecules has a strong influence on the rate of formation of surface-bound carbon monoxide and on the impact on WGS activity of the presence of co-adsorbed surface species.	Sholl, David Sievers, Carsten Chemical and Biomolecular Engineering	Jungseob So, John C Copeland, Guo Shiou Foo, David S. Sholl, Carsten Sievers

Novel Platforms and Applications

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
8.	Fadiran, Timi	Pollen as a Renewable Reinforcing Filler for Thermosetting Polymer	Pollen has the potential to be an effective filler in polymers in part due to its high mechanical strength and light weight. Pollen-polymer composites could form a new class of high-strength, light-weight materials with biorenewable filler. In this work, the effectiveness of pollen fillers in a thermosetting polymer is characterized as a function of pollen loading and surface treatment. We have found that an acid-base hydrolysis treatment of pollen can be used to tune mechanical, interfacial, and thermal properties in the thermoset. The acid-base treatment exposes and generates additional surface functional groups improving adhesion between pollen and the polymer matrix. The treated pollen is able to simultaneously stiffen and strengthen the thermosetting polymer due to its higher mechanical stiffness and the high degree of adhesion between the phases, while not significantly affecting the weight of the matrix. Thus, pollen is an attractive filler for creating high-strength, light-weight materials with a sustainable plant sourced filler.	Meredith, Carson Chemical and Biomolecular Engineering	
9.	Liu, Wei	Solar-induced direct biomass-to-electricity hybrid fuel cell using polyoxometalates as photocatalyst and charge carrier	The current polymer-exchange membrane fuel cell technology cannot directly use biomass as fuel. Here we present a solar-induced hybrid fuel cell that is directly powered with natural polymeric biomasses, such as starch, cellulose, lignin, and even switchgrass and wood powders. The fuel cell uses polyoxometalates as the photocatalyst and charge carrier to generate electricity at low temperature. This solar-induced hybrid fuel cell combines some features of solar cells, fuel cells and redox flow batteries. The power density of the solar-induced hybrid fuel cell powered by cellulose reaches 0.72 mW cm^{-2}, which is almost 100 times higher than cellulose-based microbial fuel cells and is close to that of the best microbial fuel cells reported in literature. Unlike most cell technologies that are sensitive to impurities, the cell reported in this study is inert to most organic and inorganic contaminants present in the fuels.	Deng, Yulin Chemical and Biomolecular Engineering	

Novel Platforms and Applications

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
10.	Mao, Yiqi	Anisotropic viscoplastic behaviors of mechanically fixed shape memory elastomeric composite	Shape memory polymers (SMPs) can fix a temporary shape and recover their permanent shape upon application of an external stimulus. A mechanically fixed anisotropic shape memory polymer is demonstrated theoretically and experimentally by applying anisotropic shape memory elastomeric composite (ASMEC). This ASMEC consists of an elastomeric matrix reinforced by an oriented aligned semicrystalline polymer fibrous network. By utilizing the viscoplastic property of semicrystalline fibrous mat, a temporary shape can be fixed upon unloading, since the induced unrecoverable plastic strain resists the contractile force of elastomer matrix. After heating to high temperature, the permanent shape is recovered when the oriented fibrous network evolves from crystal phases to melt. In addition, a new procedure is proposed and demonstrated to generate self-resembled curled configuration by applying a bilayer anisotropic shape memory elastomeric composite, which finds a wide potential application in ranging from drug delivery systems to biological force probes.	Qi, Jerry Mechanical Engineering	Yiqi Mao, Jaimee M., Robertson, Xiaoming Mu, Patrick Mather, H. Jerry Qi
11.	Mu, Xiaoming	Photo-Induced Bending in an Light Activated Polymer Laminate Composite	Light-activated polymers (LAPs) are smart materials that respond to light. Compared with heat, light is an instant, remote and precise stimulus that can activate polymers in a non-contact isothermal environment. The underlying chemical mechanism of the LAPs we use is bond exchange reactions (BER) that release the pre-programmed stress by rearranging the entangled polymer network. Previous researches of this polymer system explored the photo-induced applications such as generating surface patterns or folding a box from a flat sheet. However, the required loading on the flat sheet has become a limitation for the advanced applications such as self-folding. Here we develop a laminate composite that consist of two LAP layers, experiencing stress relaxation via BER, and one intermediate polymer layer, supplying the required elastic energy for the LAP layers, enabling photo-induced bending in a free-standing state. Our laminate composite design has the promising applications in the remotely triggered space structures.	Qi, Jerry Mechanical Engineering	Ph.D. student in Jerry Qi's group Xiaoming Mu, Nancy Sowan, Christopher N. Bowman, Patrick T. Mather, H. Jerry Qi

Novel Platforms and Applications

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
12.	Sekar, Ramanan	Microbial Platform for Biogeochemical Transformation of Lignocellulosic Biomass to Biodegradable Plastic	Environmental concern over non-biodegradable plastic has stimulated development of alternative clean technologies for production of biodegradable plastic. Alternative clean technologies include biosynthesis of biodegradable polymers by recombinant microorganisms genetically engineered to produce biodegradable plastic from renewable resources. The plastic industry primarily produces polymers from petroleum-based sources. Second-generation biodegradable plastics include polyhydroxybutyrate (PHB) that is produced from renewable sources such as lignocellulosic biomass. PHB therefore provides an attractive alternative to conventional plastics. The proposed biogeochemical platform for production of biodegradable plastics is based on a microbially-driven Fenton reaction that oxidatively degrades cellulose, hemicellulose, and lignin, thus avoiding use of expensive cellulase, hemicellulase, and lignolytic enzymes for lignocellulose degradation. In comparison to traditional Fenton or photo Fenton-based oxidation systems, the microbially-driven Fenton reaction operates at neutral pH and does not require addition of exogenous H_2O_2 or UV irradiation to regenerate Fe(II). Microbial Fe(III) reduction by Shewanella oneidensis replaces the requirement of UV irradiation to regenerate Fe(II) as a Fenton reagent, while the aerobic electron transport system produces H_2O_2 as a byproduct of aerobic respiration. Simple reducing sugars are the predicted primary degradation products of lignocellulose degradation from the Fenton reaction. The consolidated biogeochemical process consists of S. oneidensis-driven Fenton degradation of lignocellulosic biomass coupled to PHB production using the PHB biosynthetic cassette phaCAB of Ralstonia eutropha cloned into a recombinant, sugar-adapted S. oneidensis strain.	DiChristina, Thomas Biology	
13.	Tang, Zhenguan	Non-fluorinated organosilicon coating material for the fabrication of amphiphobic paper	A new non-fluorinated organosilicon coating material has been developed to fabricate amphiphobic paper. Paper is coated by immersing untreated paper into a coating solution for short amount of time and then dried under ambient conditions. Coating materials adhere strongly to paper surfaces by establishing siloxane bonds between cellulose fibers and hydrolyzed organosilicon molecules generated through a condensation process. Coated paper displays strong resistance towards water, diiodomethane and motor oil. Compared with existing coating materials, this new material does not contain fluorine, and is therefore more environmentally friendly than are fluorinated films. The porous structure of the paper is also largely retained after coating, which ensures flexibility and air permeability compared to other grease-proof paper. The coating process is conducted in an aqueous environment under ambient conditions at a relatively fast rate. As a result, it can be easily integrated into current paper manufacturing processes.	Breedveld, Victor Hess, Dennis Chemical and Biomolecular Engineering	

Novel Platforms and Applications

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
14.	Yang, Hua	Molecular dynamics simulation of bond exchange reaction in covalent adaptable networks	It was recently reported that covalent adaptable networks (CANs) with thermally induced bond exchange reactions (BERs) can rearrange their microscopic topology without impairing the network integrity. Besides, two pieces of polymers were shown to be able to weld together upon heating without introducing additional monomers or chemicals on the interface, enabling thermoforming, self-healing, and reprocessing of the polymer. In this study, we will use molecular dynamics (MD) simulation to investigate the molecular details of such adaptable networks. Specifically, by tracking the end-to-end distance between two neighboring crosslink sites when the BERs are undergoing, the material cross-linking density and modulus are examined. The simulation results help to understand how the polymer chains will migrate within the network, as well as across the interface to join two pieces of polymers, which provide information to further assess the network topology evolution, and describe the surface welding effect during the material reprocessing.	Qi, Jerry Mechanical Engineering	**Hua Yang, Yafang Guo, Xinghua Shi, Yujie Wei, H. Jerry Qi**
15.	Yu, Kai	1) Controlled Sequential Shape Changing Components by 3D Printing of Shape Memory Polymer Multimaterials 2) Reprocessing and Recycling of Thermoset Polymers based on Bond Exchange Reaction	1) In this study, we demonstrate d the feasibility of using the 3-D printing technique to create functional, graded shape memory polymers (SMPs) with both spontaneous and sequential shape recovery abilities. The created SMP components, with properly assigned spatial variation of the thermodynamic property distribution, react rapidly to a thermal stimulus, and return to a specified configuration in a precisely controlled shape-changing sequence. The use of the 3-D printing technique enables a manufacturing routine with merits of easy implementation, large design freedom, and high printing resolution, which promises to advance immediate engineering applications for low- cost, rapid, and mass production. 2) Recently, it has been reported that by properly catalytically controlling bond exchange reactions (BER), thermoset polymers could be welded by simple heating. This novel technology also enables us to reprocess and recycle the thermoset polymers. In this study, we experimentally demonstrated that, after being milled into pulverous state in micro-size, the thermoset epoxy polymer with exchangeable bond could be welded and assembled again into integrity with regained mechanical properties comparable to a fresh bulk polymer. Such an in-depth reprocessing routine could be repeated multiple times in the manufacture of complex objects and welding of separated bulk polymers. Considering the efficient and robust welding effect among polymer particles, as well as the maintained merits of thermoset polymer as stress-bearing materials during the operation, this new strategy is more suitable to repair polymer structures in service, and to recycle the thermoset waste in most engineering applications.	Qi, Jerry Mechanical Engineering	1) Kai Yu, Alexander Ritchie, Yiqi Mao, Martin L. Dunn, H. Jerry Qi 2) Kai Yu, Philip Taynton, Wei Zhang, Martin L. Dunn and H. Jerry Qi

Novel Platforms and Applications

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
16.	Zhang, Yi	Capillary foams: how a small amount liquid can make a big difference	Liquid foams are familiar from beer, frothed milk, or bubble baths; foams also play important roles in oil recovery, lightweight packaging, and insulation. Here we report a new class of foams, obtained by frothing a suspension of colloidal particles in the presence of a small amount of an immiscible secondary liquid. A unique aspect of these foams, termed “capillary foams”, is the particle-mediated spreading of the minority liquid around the gas bubbles. The resulting mixed particle/liquid coating can stabilize bubbles against coalescence even when the particles alone cannot. The coated bubbles are further immobilized via entrapment in a network of excess particles connected by bridges of the minority liquid. Capillary foams were prepared with a diverse set of particle/liquid combinations to demonstrate the generality of the phenomenon. The observed foam stability correlates with the particle affinity for the liquid interface formed by spreading the minority liquid at the bubble surface.	Behrens, Sven H Chemical and Biomolecular Engineering	Yi Zhang, J. Carson Meredith, Sven H. Behrens

Novel Nano-Materials

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
17.	Beatty, Brian Robert	Flexible Paper-Based Bioproducts as Substrates for 2-D Nanoelectronic Materials	The field of 2-D nanomaterials is in its infancy, yet it is becoming increasingly apparent that electronics fabricated using this class of materials are going to play a major role in the future of the industry. Two examples of these materials are graphene and dichalcogenides (e.g. MoS_2). Graphene, a 2-D crystal of carbon atoms, has a remarkable conductivity and unique electronic structure that can allow for the design of novel devices. MoS_2 is a flexible semiconductor whose bandgap can be engineered by controlling the number of stacked layers and the growth conditions. However, once these materials are grown, they need to be transferred from their growth substrate before they can be utilized in end products. A benefit to this is that it opens up opportunities to explore previously unavailable substrate materials. To this end, paper-based substrates have a variety of advantages, including flexibility, recyclability, societal pervasiveness, and very low cost. With this project, we propose methods that will allow for the transfer and characterization of CVD-grown graphene- and MoS_2-based electronic devices onto paper products.	Shofner, Meisha Vogel, Eric Materials Science and Engineering	
18.	Chang, Huibin	Carbon Fibers from Polyacrylonitrile (PAN)/Cellulose Nanocrystals (CNCs)	Carbon fibers are widely used in high-strength and low-density composite materials. Among different precursors, polyacrylonitrile (PAN) is the predominant precursor for carbon fiber production. Cellulose Nanocrystals (CNCs), which have a nearly perfect crystal structure, possess high tensile strength (up to 7.5 GPa) and high tensile modulus (110-220 GPa). By comparison, the tensile strength and modulus of PAN precursor is about 1 GPa and about 20 GPa. It is hypothesized that the incorporation of highly ordered, high-strength and high-modulus CNCs will contribute to further increase in PAN-based carbon fiber strength and modulus. The purpose of this research, therefore, is to process PAN/CNCs nanocomposite fibers and to convert them into carbon fiber. PAN/CNC nanocomposite fibers are gel-spun using dimethyl formamide (DMF). Fibers will be stabilized in air and carbonized in inert environment. Precursor fibers and their stabilized and carbonized products' properties will be systematically investigated.	Kumar, Satish Materials Science and Engineering	Huibin Chang, An-Ting Chien, Clive Liu, Po-Hsiang Wang, Bradley Newcomb and Satish Kumar

Novel Nano-Materials

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
19.	Meree, Cait	Processing-property characterization of cellulosic nanocomposite films and hydrogels produced via water-based processing methods	The objective of this research is to develop a water-based processing method for incorporating large filler loadings into nanocomposite systems. Specifically, cellulose nanocrystal/poly(vinyl alcohol) (CNC/PVA) nanocomposite aqueous suspensions and films were processed and characterized at CNC loadings up to 67 wt.% with respect to polymer concentration. Both solution suspended and freeze-dried CNCs were studied with this method. Two methods for incorporating the CNCs were investigated—solution-processing and batch-mixing of aqueous suspensions. The materials produced by these methods were characterized using rheology of aqueous suspensions and dynamic mechanical analysis of consolidated films. While the general trends in experimental data were the same, differences in properties between systems made with solution-processing and batch-mixing were observed, suggesting differences in the CNC dispersion. Overall, initial results indicate that this methodology is feasible for the production of highly loaded nanocomposites and may translate to other water-soluble and biopolymer matrices.	Shofner, Meisha Materials Science and Engineering	Caitlin Meree, Emily Fitzharris, and Meisha Shofner
20.	Mulyadi, Arie	Surface-Modified Cellulose Nanofibrils as Reinforcing Fillers in Polystyrene Composites	Cellulose nanofibrils (CNFs) have been of a great interest as potential reinforcing fillers due to their excellent physical and mechanical properties. These benefits, however, are often limited by poor interfacial compatibility, especially with hydrophobic polymer. Covalent modification on the surface of CNFs by polymer grafting is introduced to address the problem. In this study, maleated styrene block copolymers were successfully grafted on the surface of CNFs. The evidences of surface grafting were confirmed through the changes in chemical functional groups, surface wetting, and thermal stability. The influences of polymer grafting on the morphological, crystallinity, and redispersion characteristics were also evaluated. The effect of surface-modified CNFs fillers on mechanical properties of polystyrene composites was assessed and compared with those utilizing neat CNFs. The preliminary results of this study provided a positive indication of CNFs as reinforcing fillers in hydrophobic polymers and the importance of CNFs surface modification for nanocomposite application.	Deng, Yulin Chemical and Biomolecular Engineering	Mulyadi, Arie; Deng, Yulin

Novel Nano-Materials

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
21.	Rosu, Cornelia	Protein-assisted active electronics incorporating semiconducting polymers on flexible and foldable cellulose substrates	Printed, flexible electronics have gained attraction as low-cost, "disposable" substitutes for conventional semiconductor devices in electronic control and monitoring for a variety of industries and applications including health care, environmental quality, national security and system integrity. A critical materials element of such devices is the semiconducting polymer which may enable application of flexible devices in technologies such as sensors, RF-IDs and photovoltaics. Paper electronics using P3HT by printing invites the use of other environmentally friendly ingredients to deliver the polymer to the paper substrate. A creative approach uses *Cerato ulmin*, a natural Janus-like protein to encapsulate and deliver P3HT. The encapsulation of P3HT solutions in the hydrophobin-stabilized, nominally cylindrical structures will improve molecular alignment for better charge transport in the fibrils which results as the organic solvent is removed. It is hoped that additional improvements to P3HT alignment, and therefore improvements to conductivity, can be brought about by also incorporating functionalized cellulose nanotubes in the structures stabilized by *Cerato ulmin*.	Reichmanis, Elsa Chemical and Biomolecular Engineering Russo, Paul S. Materials Science and Engineering	Cornelia Rosu, Elsa Reichmanis, Paul Russo
22.	Sharma, Sudhir	High Performance Cellulose Nano Fiber Composites	Presented in this study are composite membranes made from cellulose nano fibers, cellulose nano crystals, high aspect-ratio crumpled graphene sheets, and high aspect-ratio clay (magnesium silicate hydroxide). Here, cellulose nano fibers were used as the matrix and a 1% loading of the reinforcing materials was used. The membranes were made by an ultrafiltration process followed by high-pressure compression and subsequent drying under a compressive load at 75^{o}C. By this method, films with a high degree of uniform dispersion and dimensional uniformity can be obtained, which is a significant enhancement over composite membranes made from solvent evaporation methods. Composite membranes showed as much as 50% improvement in strength and as much as 100% high elongation at break as compared to pure cellulose nano fiber membranes.	Deng, Yulin Chemical and Biomolecular Engineering	

Novel Nano-Materials

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
23.	Sun, Qining	Xylan Reinforcement on Cellulose bionanocomposite film	The ever-increasing global demand for materials and international dependency on conventional petroleum resources plus the environmental concern call for alternative sustainable sources and greener technologies. In this study, novel films were prepared by depositing xylan on poplar cellulose nanowhiskers via pH adjustment. The mechanical properties, water-vapor transmission properties, surface morphology and chemical components of the films were evaluated and characterized using tensile testing, wet-cup method, AFM, 3D Opto-digital Microscope and HPAEC-PAD under controlled temperature and humidity conditions. Addition of 8% xylan improved the film tensile strength to the largest extent, increasing the tensile strength by 90 %. In addition, pH-adjusted films were significantly better at improving physical properties than the controlled group without pH adjustment.	Ragauskas, Art Chemistry and Biochemistry	
24.	Zhang, Xiaodan	Solid-State, Flexible, High Strength Paper-Based Supercapacitors	Supercapacitors are one of the main energy storage devices and are key technological enablers ranging from transportation to consumer electronics. Compared to their competitors—batteries—supercapacitors have superior cycling life, higher power densities, faster charge and discharge rates. But most of the supercapacitors are liquid-based, which gives them a lot of challenges such as the sealing problems and space constraints. Here we report a solid-state, flexible, high-strength, environmentally-friendly paper-based supercapacitor made mainly by micro-fabrillated cellulose(MFC) and multi-walled carbon nanotubes(MWCNT). The specific capacitance of such supercapacitors is calculated to be 309mF/cm^2 from cyclic voltammetry. This value is significantly higher than most flexible supercapacitors reported in literature. The paper-based supercapacitors have excellent mechanical properties, with tensile strength being 1MPa and Young's modulus being 123MPa. Moreover, the specific capacitance remained the same when the supercapacitors were bent under different curvature.	Deng, Yulin Chemical and Biomolecular Engineering	

Process Improvement

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
25.	Baykal, Bedi Aydin	Erosion-corrosion and flow effects in evaporators	The kraft pulping cycle is home to a number of corrosion concerns, not least the digesters and evaporators, where flow rate and presence of hard particles causes a form of electrochemical corrosion enhanced by mechanical effects, called erosion-corrosion. No surface is perfectly smooth, and formation of eddy currents and/or other impingements such as elbows will direct the flow of hard particles toward the vessel walls, interfering with film repassivation and causing active corrosion when it would normally not happen without the particles. Therefore, a distinctive "ice cream scoop" type of corrosion is formed behind the source of impingement. In this study, a fluid mechanics and electrochemistry approach will be used to determine the mechanism of this phenomenon and study the effects on different steels commonly used in evaporators in the pulp and paper industry, including carbon, stainless and duplex stainless steels at different flow rates and particle contents in a white liquor environment.	Singh, Preet Materials Science and Engineering	
26.	Choi, Won Tae	The Creation of Liquid Repellent Stainless Steel Surfaces	The design of liquid repellent surfaces has attracted much attention due to the potential for self-cleaning, drag reduction, or anti-corrosion applications. Despite recent significant developments, relatively few studies have been reported on the creation of liquid repellent metal and metal alloy surfaces. Here, we discuss a method to control the surface topography of stainless steel by electrochemical methods. The relative etch-rate between grains and grain boundaries was controlled by the bias potential applied to the stainless steel, thereby permitting variation of the surface topography. With the application of a low potential (1.0V), high selectivity between grain and grain boundary etching was achieved, which resulted in significant grain boundary etching. As the potential was increased, etch selectivity decreased and ultimately generated smooth, electro-polished surfaces. Using contact angle measurements, the wetting behavior of etched stainless steel surfaces was determined and related to the specific topography created by the electrochemical treatments.	Breedveld, Victor Hess, Dennis Chemical and Biomolecular Engineering	Won Tae Choi, Kkochnim Oh, Preet M. Singh, Victor Breedveld, Dennis W. Hess

Process Improvement

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
27.	Collins, James Ruschau, Alex	Strain Field Mining and Paper Strength	Strain field mining is a new analysis strategy that uses spatial statistics to extract critical information from strain maps in deforming paper. Originally developed to predict the performance of polymer adhesive bonded joints, we are extending our data-mining approach to enable improvements in the mechanical performance-to-weight ratio of paper. In this poster, we present the tensile strength, stiffness, and energy absorption (per TAPPI T 494) of a copy paper as a function of orientation. The results from standard cut strip specimens showed higher variability and near-grip failure data rejection rates than a dog-bone geometry adapted from ASTM E E345. The compliance-corrected tensile deformation behavior of the two tensile specimen geometries is also compared to the constitutive response measured using full-field strain mapping.	Muhlstein, Christopher Materials Science and Engineering	James Collins, Alex Ruschau, Christopher Muhlstein
28.	Du, Xiaotang	Adsorption deinking and electric treatment for microstickies agglomeration	Adsorption has been used to improve inkjet inks removal during pulping. Chitosan was found to be an adequate adsorbent, which was able to remove 50%-70% of ink from an ink/water solution in 30 min. Adsorption deinking efficiency was significantly better when the pulping consistency was reduced from 15% to 10%. The ISO brightness and ERIC were deinked to above 54 and below 300, respectively. Microstickies could deposit on both paper machine and paper products, especially after agglomeration under shocks in ionic strength, pH, temperature and chemical additives. The most important property of microstickies is the small size, leading to low removal efficiency and difficulties in measurement. A new agglomeration technology based on electric field is investigated that can increase the particle size from less than 1 micron to over 10 microns. The synergetic effect between electric field treatment and detacky chemicals/dispersants, including polyvinyl alcohol (PVA), poly(diallylmethylammonium chloride)(PDADMAC), lignosulfonate, are also studied.	Hsieh, Jeff Chemical and Biomolecular Engineering	

Process Improvement

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
29.	Dutzer, Michael	Residual Metal in Titanium Carbide-Derived Carbon for the Adsorptive Removal of VOCs	Volatile organic compounds (VOCs) are produced in many chemical processes and can cause harm to human health and the environment. Novel removal methods, including adsorption processes, are under development to remediate the potential harm caused by VOCs and to provide the potential for new revenue streams through chemical feedstocks from waste streams. Carbide-derived carbons (CDCs) offer one such solution. CDCs are porous carbons derived from metal carbides with high surface area, controllable pore-size distributions, and chemical and thermal stability. CDCs are produce by selectively removing the metal atoms from a metal carbide using a high-temperature etching process. This selective removal of metal atoms leaves behind a narrow distribution of pore sizes in a carbon complex. Complete metal removal shows enhanced adsorption of VOCs, such as methanol, over current technology; however, this has the potential for further improvement through partial or incomplete etching. The residual metal serves as active adsorption sites that improve the functionality of the CDC by allowing for a stronger adsorption process. Partial etching and post-etching modification negates the need for metal doping required by other activated carbons because the metal is present initially in the precursor. Titanium has been shown to catalyze methanol and formaldehyde in the reduced metal state, while titanium dioxide has been shown to photo-catalytically destroy both VOCs. Based upon these metal-to-VOC interactions, titanium carbide-derived carbon (TiCDC) has excellent potential to be tuned for the adsorptive removal of methanol and formaldehyde.	Walton, Krista Chemical and Biomolecular Engineering	
30.	He, Liang	Scanning Electrochemical Microscope (SECM) in the Research of Localized Corrosion Behavior	Electrodes with millimeter dimensions are used in the majority of electroanalytical measurements. This kind of electrode collects voltage and current perturbations over the whole samples. However, for localized corrosion such as pitting and crevice corrosion, there is only intense attack at localized sites on the surface, while the rest of the surface is under satisfactory corrosion control. In this case, electrodes with millimeter dimensions cannot capture the behavior of localized corrosion sites. To overcome this problem, ultramicroelectrodes (UME) with at least one dimension in the micrometer range were invented. Scanning electrochemical microscope (SECM) utilizes UME as probe, greatly increasing its spatial resolution. In this study, the microstructure of duplex stainless steels and the sites for localized corrosion were characterized by SECM using generation/collection mode, which creates better understanding of the mechanism for localized corrosion.	Singh, Preet Materials Science and Engineering	

Process Improvement

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
31.	Howell, Aaron	Computational Simulations of Black Liquor Falling Film Evaporation	Falling-film evaporators are today the dominant technology for black liquor concentration. During evaporation, differences in concentration of the liquid film cause diffusion-driven mass transport. As the water is evaporated, various salts, especially sodium carbonate and sodium sulphate, will exceed their solubility and crystallize. Understanding these processes is key to obtain high reliability and availability in black liquor evaporation plants. The computational simulation is achieved by solving the conservation of mass, momentum, energy, and species. The methods used are able to render the complex interaction at the free surface between black liquor and vapor. Additional features include the ability to describe heat transfer to the black liquor, evaporation of black liquor causing dry solids enrichment, and black liquor rheology. Presented are the results for black liquor up to 65% dry solids. Complex three-dimensional free surface waves are captured by the computational model.	Aidun, Cyrus Mechanical Engineering	
32.	Hume, Chad	Design and Analysis of Press Fabric Structures for Improved Dewatering	During paper manufacturing, one of the main energy consumers is drying the paper web. Energy consumption could be greatly reduced if web dewatering efficiency could be improved. The current work explores methods for increasing dewatering efficiency in press fabrics. Specifically, a systematic investigation was conducted of water flows in press fabrics through computational fluid mechanics (CFD) with the objective of designing geometric features that aid dewatering. Various hole designs are studied to understand which features aid dewatering and, possibly, act as check valves to prevent water reabsorption as pressure is released after passing through the nip. Circular, elliptical, and other cross-section shapes are investigated, as well as 3-D conical and grooved shapes. Hole sizes range from 10 mm to 2 mm. Result show improved resistance to back flow when compared with traditional press fabric base layer geometry.	Rosen, Dave Mechanical Engineering	

Process Improvement

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
33.	Kevlich, Nikita Sergeevich	Concentration of Kraft Black Liquor via Carbon Molecular Sieve Membranes	Large amounts of energy are required for the concentration of black liquor (BL) by multiple-effect evaporation in the Kraft papermaking process. Membranes have the potential to significantly reduce this energy consumption. However, current membranes are not sufficiently robust under the harsh black liquor conditions (pH>10.5, 80-90°C, high fouling), and do not have high enough performance. The goal of this project is to design carbon molecular sieve (CMS) membranes that overcome these limitations. Free standing CMS membranes have been synthesized by pyrolyzing polymeric membranes under vacuum. The membranes were found to be stable in BL up to pH 12 at 90°C. Nitrogen physisorption measurements showed that these CMS membranes have a high surface area (~600 m^2/g) with majority of pores in the micropore region (<2 nm). Upcoming work will involve detailed membrane permeation measurements in a reverse osmosis system with both simulated and real BL feeds.	Nair, Sankar Chemical and Biomolecular Engineering Shofner, Meisha Materials Science and Engineering	**Ketki Sharma, Nikita Kevlich, Meisha Shofner and Sankar Nair**
34.	Liu, Yitao	Optimal Resource Balancing and Factory Loading for Energy Cost Reduction in the Pulp and Paper Industry	Pulp and paper manufacturing has been known to be one the largest industrial sector consumers of energy. The needs of energy cost saving is compelling due to the increasing volatility of energy prices in today's marketplace. The challenge of maintaining high product quality while simultaneously reducing production costs can often be met through investments in energy efficiency, which can include the purchase of energy-efficient technologies and the implementation of plant-wide energy efficiency practices. In this research, a technical framework of system modeling technique is introduced to model energy conversion and utilization throughout the pulp and paper manufacturing system and sub-systems. A well-established SysML-based process model is translated to a Discrete-Event Simulation model. By simulating the system's response to the changing energy price and market demands, diverse *what-if* scenarios of system energy utilization can be analyzed in terms of reduction of the total energy cost.	Jiao, Jianxin (Roger) Mechanical Engineering	Yitao Liu, Roger J. Jiao

Process Improvement

	Name	Title	Abstract	Advisor/Schools	Notes/Authors
35.	Oh, KkochNim	Effects of Ni on the Localized Corrosion and Repassivation Kinetics of Fe-20Cr-xNi (x = 0~20 wt. %) Stainless Steels	Ni, a structure-determining element in SSs, is found to have a significant influence on the susceptibility to stress corrosion cracking (SCC) in a hot chloride solution. According to the well-known Copson diagram, te-20Cr-xNi alloys (x=0~80 wt. %) exhibited the maximum susceptibility to chloride SCC at 10 wt. % Ni. Since SCC of SS in chloride solution occurs by repetitive processes of film breakdown/dissolution/ repassivation, we examined the effects of Ni on the film breakdown, repassivation kinetics and dissolution processes of the alloys respectively, to elucidate the influences of Ni on SCC of Fe-20Cr-xNi (x = 0~20 wt. %) SSs. It was found from electrochemical noise tests that Fe-20Cr-10Ni SS exhibited the maximum susceptibility to metastable pitting corrosion. It appears that the maximum susceptibility of Fe-20Cr-10Ni SS to metastable pitting corrosion is associated with the highest defect density in passive film of the alloy such as oxygen vacancy and/or metal ion vacancy, as measured by the Mott-Schottky analysis for the film of the alloys. Repassivation kinetics of the alloys was examined using the rapid scratch electrode test. The repassivation rate of Fe-20Cr-xNi (x = 0~20 wt. %) SS was increased with an increase or a decrease in nickel content from 10%, confirming that the repassivation rate of Fe-20Cr-10Ni SS is the lowest among the alloys. It is evident, from the similarity in the effects of nickel on SCC (Copson diagram) and also on the repassivation rate of the alloys, that the susceptibility to SCC of the alloys is determined by their repassivation rate. Anodic dissolution process at crack tip was simulated by an occluded corrosion cell test in which a small anode in deaerated acidified chloride solution is connected galvanically to a large cathode in aerated chloride solution via a zero-resistance ampere meter. Anodic dissolution rate in the small anode in the occluded cell test decreases with an increase in nickel content of the alloys, demonstrating that crack growth rate of Fe-20Cr-xNi SSs would be decreased with nickel content.	Singh, Preet Materials Science and Engineering	

Process Improvement

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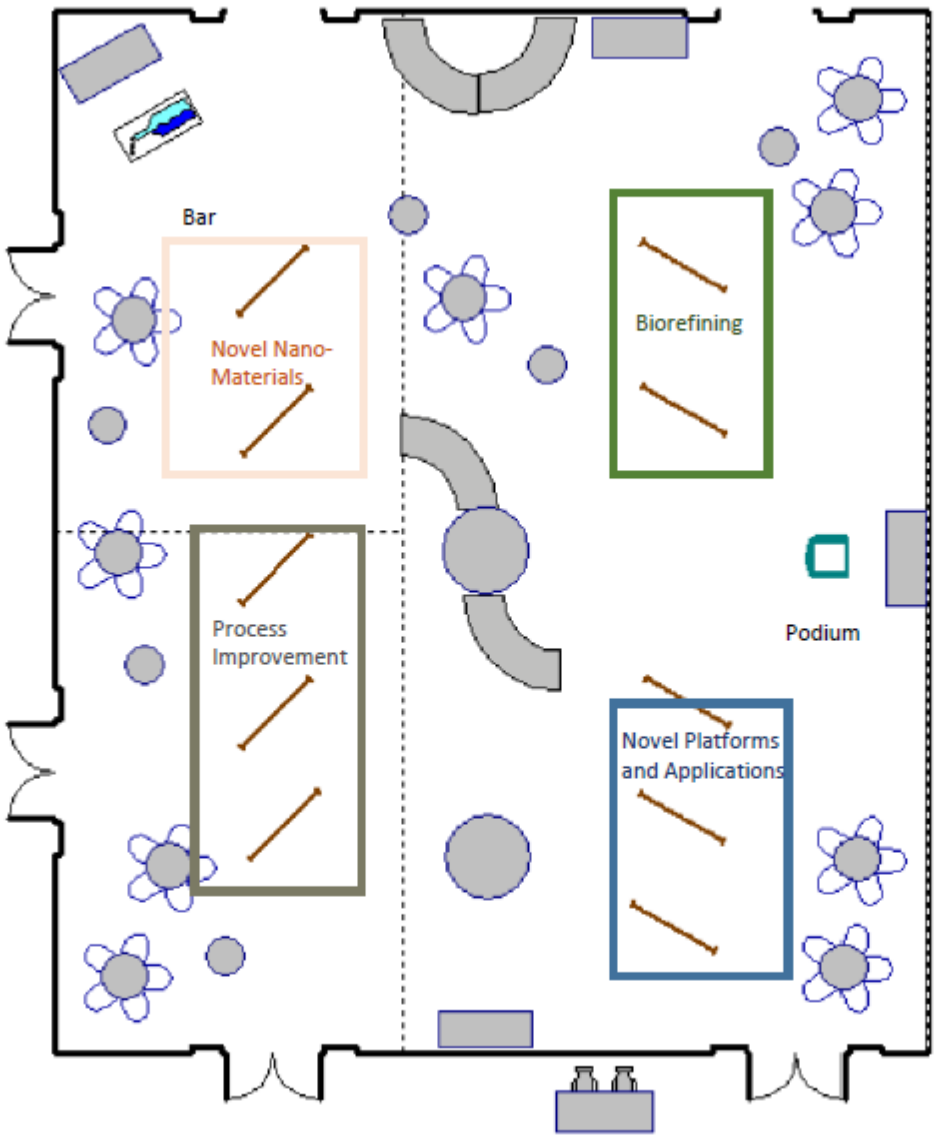
36.	Wang, Yushu	Thiosulfate pitting of stainless steels in paper machine white water	Thiosulfate pitting of stainless steels has been a corrosion concern in paper machine white water environment. Thiosulfate is a by-product of bleaching agent. It promotes pitting by inhibiting repassivation of pits. Regulations and constraints on water usage and wastewater discharge lead to reductions in effluent volumes through reuse of process water and of treated wastewater, which increases the chemical concentrations in white water and may aggravate the corrosion issue. Local concentrations of chemicals may also increase due to water evaporation. In this study, the effect of white water chemistry and concentration of white water on thiosulfate pitting on austenitic stainless steels as well as duplex stainless steels is investigated.	Singh, Preet Materials Science and Engineering	



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