Computation-Ready Experimental (CoRE) Metal-Organic Frameworks: A Critical Tool to Enable High-throughput Screening of Nanoporous Crystals

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Metal-organic frameworks (MOFs) are a class of crystalline nanoporous materials with record surface areas and unique pore geometries. Computational screening of the over 6,000 experimentally reported MOF structures can streamline efforts to identify materials suitable for applications ranging from gas storage to chemical sensing. These computational screening efforts depend on simulation-ready crystallographic information for each structure. To date, the availability of simulation-ready crystal structures is a major impediment to applying high-throughput computations to MOFs because experimentally refined structures include artifacts such solvent molecules that significantly decrease porosity. The central result of this work is the public availability of a nearly comprehensive set of MOF structures that are derived directly from experimental data but are immediately suitable for molecular simulations. As an example of using our CoRE MOF database, we have determined the storage capacity of adsorbed natural gas in vehicle fuel tanks based on over 4,000 different porous MOF materials.
Optimization of Pollen Performance as a Filler in Polymer Composites

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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. Due to pollen’s unique architectures, these composites also provide insights to how filler microstructure may affect wetting and adhesion between phases. In this work, the effectiveness of pollen fillers in polyvinyl acetate and epoxy matrices is characterized as a function of pollen loading. We have found that different surface treatments of pollen can be used to tune mechanical, interfacial, and thermal properties in both matrices. In epoxy, pollen becomes a load bearing filler after acid-base hydrolysis. In PVAc, pollen becomes a load bearing filler after an additional functionalization with a silane coupling agent. Pollen is more compatible with epoxy than PVAc, due to hydrogen bonding between epoxy and pollen.
Surfactant-Mediated Electric Charging Mechanisms in Nonpolar Media

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Electric charging in nonpolar media is much less common than that in aqueous media because of the large energetic cost of sustaining charges in such low dielectric media. It is nonetheless observed in the presence of surfactant additives and is important in a wide range of applications. The precise mechanisms are yet poorly understood since only a small number of vastly different commercial surfactants have been investigated without addressing the impurities. The present work investigates the electric charging of polymeric particles mediated by a series of custom-synthesized and well-purified polyisobutylene succinimide (PIBS) polyamine surfactants with small structural variations. Conductivity and electrophoretic mobility measurements assessing the charging effect of the surfactants are complemented by light scattering studies of the surfactant micelles. Acid-base interactions between the particle surface and the surfactant are studied quantitatively by interfacial tensiometry and contact angle measurements.
High Sensitivity, Positive Tone, Low-k Polynorbornene Dielectric

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In microelectronics packaging, low-k dielectrics are used to mechanically and electrically isolate conductive interconnects. Positive tone, aqueous developable, polymeric dielectrics are used for this purpose due to their high yield, environmentally friendly, and high throughput processing. Furthermore, these materials must have excellent mechanical and electrical properties, which typically require cross-linking of the polymeric film. Positive tone chemical amplification can provide high photospeed and contrast, but the photo-generated acid necessary for patterning also catalyzes cross-linking reactions.

Presented in this work is the first chemically amplified, positive tone, cross-linkable dielectric. The base polymer is polynorbornene with pendent fluoroalcohol and tert-butyl ester moieties. This polymer is successfully patterned at photospeeds > 10x faster than existing materials. After photolithography, the dielectric is cross-linked via a Fischer esterification. The resulting film had a modulus of 2.99 GPa and a dielectric constant of 2.78, both very promising for its use in microelectronics.
Directed Self-Assembly of Block Copolymers: Enabling Materials and Process Development for Semiconductor Patterning using Molecular Simulation

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Continuation of Moore’s Law device scaling in semiconductor manufacturing faces a number of challenges, the greatest of which is developing methods for printing sub-40 nm pitch patterns required for future device fabrication. Directed self-assembly (DSA) of block copolymers, in which lithographically produced templates are used to guide the natural microphase separation behavior of block copolymers to form ordered patterns over large areas on surfaces, is a very promising new method for achieving such small patterned features. One alignment template method, referred to as chemoepitaxy, utilizes chemical gradients on the substrate surface to register, align, and provide long range order in the block copolymer patterns. This presentation will review the development and use of molecular simulation methods for: (1) predicting the behavior of block copolymer phase separation processes and (2) rapidly designing materials and processes to achieve sub-20 nm pitch DSA with low defectivity.
High Performance Green Barrier Films from Thermal Treatment of Cellulose Nanofibrils

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Hornification due to thermal exposure has been shown to be detrimental to the properties of cellulose fibers and the formation of paper. This is due to closure of pores, reduction in hydrophilic nature of fibers due to irreversible hydrogen bonding of the –OH groups of the fibers and increased crystallinity. However, these effects of thermal exposure could be very beneficial in the enhancement of barrier properties of membranes made from Nanocellulosic fibers (NCF) fibers for oxygen and water vapor. In this study we demonstrate that controlled thermal exposure (heat treatment/annealing) after forming membranes from NCF fibers can indeed enhance the barrier properties of these membranes. We demonstrated 3 hours of thermal exposure (at 175°C) to films of about 75μm thickness results in the improvement in oxygen barrier by almost 25 fold while water vapor permeability could be reduced to half, while being accompanied by all the consistent hornification changes. The films were found to be decreasing in porosity with increasing heat treatment temperature. The oxygen and water vapor permeability reduced from 0.17 to 0.007 (ml.μm/m2.day.kPa) and 3.12 to 1.544 (kmmol.μm/m2.day.kPa) respectively. Thermal exposure to the films was also accompanied by expected hornification effects, closure of porous structure, increase in size of crystallites by more than 45% (0.067 – 0.099nm) increase in hydrophobicity increase in contact angle from 64° - 96° and decrease in water retention value by more than 55%. This study shows that the barrier and mechanical properties of films made from NCFs can be fine-tuned by controlled thermal exposure.
Impact of Air Exposure on Adsorption in MOF-74

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MOF-74 is a widely studied metal organic framework (MOF) that can be synthesized isostructurally with different metals, commonly magnesium, cobalt, nickel, and zinc. Upon solvent removal and activation, these metals are coordinatively unsaturated, leaving desirable sites for adsorption. Mg-MOF-74 has shown very high equilibrium CO₂ capacities, and Co-MOF-74 and Ni-MOF-74 are quite promising for carbon monoxide adsorption. However, the ideal handling and storage conditions required to achieve record capacities may not be practical on a large scale. These conditions include a loss of accessible surface area after short-term exposure to ambient air, leading researchers to store samples under solvent or inert. In this work we look at the impact of air exposure on the equilibrium and dynamic carbon monoxide adsorption in Mg-, Co-, and Ni-MOF-74 in order to quantify the impact on capacity to guide future work with these promising materials.
Encapsulation of Gold Nanoparticles in Stable Metal-Organic Frameworks

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Metal-organic frameworks (MOFs) are porous, crystalline materials with the potential for applications in gas storage and separation, air purification, and catalysis. They provide advantages over other porous materials due to their high surface areas and pore volumes, uniform pore size distributions ranging from micro to mesopores, and chemically functionalized sorption sites. Unfortunately, for target applications such toxic gas removal, the MOF needs to be stable under humid conditions. There are several MOFs known to be stable under humid conditions; however, they do not sufficiently interact with toxic gases such as carbon monoxide or ammonia. However, doping these MOFs with metal or metal oxide nanoparticles can significantly improve adsorption and catalytic abilities. Gold nanoparticles are particularly attractive because of their low temperature catalytic capabilities of toxic gases such as CO. This presentation will introduce work on encapsulating gold nanoparticles in stable metal organic frameworks.
Solvent-Assisted Directed Self-Assembly of Block Copolymers: Understanding Fundamentals of Solvent Uptake in Polymers

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Lithographic patterning methods used for integrated circuit fabrication have reached their limits. Microphase separation of block copolymers into structures with characteristic length scales on the order of 10 nm is a promising alternative to conventional lithography. In particular, use of lithographically derived guiding templates to provide order and registration of block copolymer patterns via “directed self-assembly (DSA)” methods is promising. DSA methods require that the block copolymer film be annealed above its glass transition temperature (Tg) to allow for ordering of the film. Use of solvent annealing is attractive since it can allow for plasticization of the film to below room temperature and is generally applicable to all block copolymers. This work presents fundamental studies aimed at providing thermodynamic data and rules that can be used to properly select solvent and annealing conditions for such DSA processes.
Development of Reactive Chromatography Systems for Equilibrium-limited Reactions

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Reactive chromatography is a process that combines reaction and separation in a single unit that leads to a greater process performance. This process is especially advantageous when the reaction is equilibrium limited, and the in-situ separation of products shifts the equilibrium in the direction of conversion increase. In the present work, we study the application of reactive chromatography to the synthesis of an ester using AMBERLYST™ 15 as a catalyst and adsorbent. This study focuses on the production of propylene glycol methyl ether acetate, one of the most commonly used esters with a high industrial demand. In this presentation, a case study of process development for the ester product is discussed. Kinetic parameters and their dependence on temperature were determined by fitting the model to the experimental data. In addition to the development of model, the feasibility and efficiency of reactive chromatography where the conversion exceeds the reaction equilibrium of the batch reaction were demonstrated.
Diffusion of Hard and Soft Colloids Trapped Between Parallel Walls

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We will present experimental studies of Brownian diffusion of hard and soft colloids under confinement between parallel walls via particle tracking video microscopy. The presence of a solid wall imposes constraints on the flow field and affects the mobility of a particle by hydrodynamic coupling. Our objective is to study the effect of softness on hindered diffusion and determine the parameters that distinguish soft from hard colloids. Polystyrene beads were used to model hard colloids and toluene-swollen polystyrene beads were used as incompressible, deformable soft colloids. We observed that the confinement behavior of the swollen beads depends on the presence of surfactant, nature of the confinement surface, swelling ratio of the swollen beads. These experiments show that the behavior of swollen polystyrene beads under confinement can be significantly different from hard colloids. Future work will focus on the confinement of the microgels, which are both compressible and deformable.
Optimization Based Design and Experimental Validation of Simulated Moving Bed Chromatography Systems for Ternary Separation

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Simulated moving bed (SMB) chromatography is an adsorptive separation process where the components are separated utilizing their varying affinity towards the stationary phase. Over the past decade, many modifications have been proposed in the SMB chromatography in order to effectively separate a binary mixture. However, the separation of a multi-component mixture using SMB is still one of the major challenges. In this study, we have compared various existing ternary separation operating strategies in terms of the maximum throughput attained. In addition, we have also found Generalized Full Cycle strategy, based on a systematic design, which is found to have significant improvement over existing operations. We are currently working on experimental validation of the operating strategies. A prediction-correction method has been implemented to arrive at optimal operating conditions which stratifies the optimal throughput as well as the desired purity and recovery of the products experimentally.
Preliminary research into poly(ethylene furanoate) (PEF), a recently developed furanic and biologically-sourced analog to poly(ethylene terephthalate) (PET), has shown that PEF is superior to PET in regards to thermal, mechanical, and barrier properties. The current work provides a detailed oxygen transport investigation using pressure-decay sorption and permeation techniques at various temperatures. Detailed sorption measurements using a high accuracy custom-built system will be presented, along with so-called dual-mode sorption parameters for oxygen, which has very low sorption uptake in PEF. The validity of the resultant sorption parameters is demonstrated through complementary and independent permeation measurements. Furthermore, the energetic parameters associated with the oxygen transport process (i.e. enthalpy of sorption, activation energies of permeation and diffusion) are presented for PEF. This study is the first detailed investigation of oxygen transport in PEF, and in combination with our prior work, illustrates the property improvements for PEF vs. PET.
A New Regime for Carbohydrate Chemistry?
High pH Dimerization of Glyoxylate

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At pH 14 under aqueous conditions, cyanide catalyzes the dimerization of glyoxylate to form dihydroxyfumarate (DHF) followed by a hydroxide-promoted aldol reaction-fragmentation process between DHF and glyoxylate producing tartrates in high yields. A mechanism for these transformations is provided and is supported by NMR measurements using isotopically labelled reactants. The selectivity of this reaction pathway and stability of the products at these conditions contradicts the conventional wisdom that highly basic conditions are prohibitive to carbohydrate chemistry, and may in fact indicate promising conditions for conversion of biological feed stocks.
Solid Phase Reactive Simulated Moving Bed Chromatographic Separation System for Biofuel Production

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A new reactive separation process concept termed solid-phase reactive separation system (SPRSS) is proposed. SPRSS integrates the progressing batch reactor (PBR) and simulated moving bed (SMB) chromatography concepts. This process concept is applied to the production of sugar from lignocellulosic material using concentrated acid hydrolysis. Both PBR and SMB employ similar principles of the movement of the liquid feed to imitate the countercurrent movement of solid and liquid phases. The overarching goal is to improve the sugar yield and sugar product concentration while minimizing the sugar decomposition reaction and undesired product formation. Moreover, the acid consumption is expected to be further reduced and therefore decrease the cost of acid recycle. An optimization strategy using a superstructure formulation will be applied to find the optimal process parameters and process configurations of SPRSS.
A Novel Chemical Pretreatment Method to Accelerate Bioconversion Rate of Renewable Feedstocks for Biofuel Applications

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Lignocellulosic biomass is the most abundant naturally renewable organic resource for biofuels production. Due to its recalcitrance to hydrolysis, pretreatment is a crucial step prior to enzymatic hydrolysis of the feedstock. A variety of pretreatment methods have been intensively studied to achieve optimal yield without imposing significant adverse impact on the environment. Herein, we present a novel chemical pretreatment method using substituted heterocycles.

1-Methylimidazole is a precursor to some imidazolium-based ionic liquids. It can be used as a pretreatment agent at mild conditions to obtain a substantial increase in the hydrolysis rate. Besides, 1-methylimidazole was found to be an effective delignifier for a variety of plant biomass such as untreated and steam-exploded loblolly pine, switchgrass and sugarcane bagasse. The mechanism of 1-methylimidazole pretreatment is investigated through analysis of cellulose physical properties including crystallinity index, degree of polymerization, accessibility as well as lignin dissolution quantification and lignin characterization.
Poly(ethyleneimine) Infused and Functionalized Torlon®/Silica Hollow Fiber Sorbents for Post-Combustion CO₂ Capture

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Organic-inorganic hybrid materials functionalized with amine-containing reagents are emerging as an important class of materials for capturing carbon dioxide from flue gas. Polymeric/silica hollow fiber sorbents are fabricated through the proven dry-jet/wet-quench spinning process. In our study, a new technique for functionalizing polymeric/silica hollow fiber sorbents with poly(ethyleneimine), followed by a post-spinning infusion step was studied. This two step process introduces a sufficient amount of poly(ethyleneimine) to the polymeric/silica hybrid material support to improve the CO₂ sorption capacity due to the added amine groups. The poly(ethyleneimine) infused and functionalized hollow fiber sorbents are also characterized by a thermal gravimetric analyzer (TGA) to assess their CO₂ sorption capacities.
Nodular-Skinned Hollow Fiber Membranes for Carbon Dioxide Capture via Sub-Ambient Temperature Operation

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Increasing atmospheric CO₂ concentration has been suggested as a factor causing climate change. A large percentage of CO₂ emission is attributed to pulverized coal (PC) power plants. Post-combustion flue gas CO₂ capture is a challenging application, but it has the greatest near-term potential for implementation. Our work considers the capture of CO₂ at sub-ambient temperatures using Matrimid® asymmetric hollow fiber membranes. Membranes with special nodular skin morphology have been successfully formed in this work. Compared to integrally defect free membranes, the nodular-skinned membranes display higher productivity and higher separation efficiency at sub-ambient temperatures, as well as good mechanical strength and tolerance for trace amount of water.
Influence of Pyrolysis Conditions on Gasification of Biomass Chars Formed in an Entrained-Flow Reactor

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Any lignocellulosic biomass can be converted to syngas by gasification. Conversion of syngas to fuels/chemicals requires high pressures. High-pressure gasification prevents the need for the costly compression step for subsequent fuel/chemical synthesis applications of syngas. Flash pyrolysis (heating rate $10^3$-$10^4$ K/s) of pine was performed in a pressurized entrained flow reactor (PEFR) at 873-1273 K and 5-20 bar. Slow pyrolysis (~10-50 K/s) of pine was performed in a PTGA at 800 °C between 5-30 bar.

Pyrolysis conditions have a drastic impact on the release of major gases (CO, CO$_2$, H$_2$, CH$_4$), C$_2$-C$_4$ hydrocarbons, light oxygenates and tars. Gas phase free radical repolymerization reactions are considered as a plausible route for tar formation. The gasification activity of chars, using CO$_2$ and H$_2$O as gasifying agents, is found to be dependent on micropore surface area, nature of carbon (amorphous vs. graphitic), ash content, ash composition and distribution within the char matrix.
Nitrogen/Methane Separation Using Carbon Molecular Sieve Membranes

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Membrane separation is an attractive alternative to remove nitrogen from natural gas compared to other technologies due to its high energy efficiency and high adaptability. However, the small size difference between nitrogen and methane and the competing effects between diffusion and sorption lead to unattractive permselectivity using traditional polymeric materials. Carbon Molecular Sieve (CMS) membranes overcome this problem by providing a hyper-rigid structure and distinctive bimodal pore size distribution. The separation performance of CMS membranes derived from a series of polyimides and polyamide-imide, as well as the optimization during pyrolysis process will be presented. Several CMS samples have shown attractive nitrogen/methane separation performance well above the polymeric membrane upper bound line. A strong molecular sieving effect is achieved by a very tight 'slit-shaped' pore structure that can effectively distinguish the size and shape difference between nitrogen and methane.
Petroleum is diminishing in supply, and it is important to find alternative feedstocks to produce transportation fuels. Flash pyrolysis of biomass is one method of fuel production, but the resulting product mixture has many unfavorable characteristics which can be resolved using hydrodeoxygenation (HDO). The two main requirements for HDO catalysts are the presence of defect sites to bind oxygenates and the ability to adsorb and dissociate hydrogen. Defects site formation is characterized with temperature-programmed reduction (TPR) as well as temperature-programmed oxidation (TPO). Hydrogen-deuterium (H₂-D₂) exchange, at varying hydrogen and deuterium concentrations, is used to understand the kinetics of dissociative adsorption of hydrogen. Infrared spectroscopy is used to examine the types of hydroxyl groups involved in isotopic exchange. The work presented here examines the necessary requirements for HDO in metal free mixed metal oxides. The catalysts’ properties are characterized and correlated with reactivity data to determine methods for catalyst design.
Novel Thermo-responsive Ligands for Glycoprotein Purification by Affinity Precipitation

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Novel thermo-responsive carbohydrate-affinity ligands were developed by fusing a bacterial fucose lectin with a thermo-responsive polypeptide. These designer affinity ligands fusions were produced using an E. coli system capable of extracellular secretion of recombinant proteins and were isolated with a high recovery yield (95%) directly from growth medium by Inverse Temperature Cycling (ITC). Using horse radish peroxidase (HRP) as a model protein, the designer thermo-responsive ligands interactions are demonstrated with glycans on a glycoprotein. This property was then used to develop a novel affinity precipitation method for glycoprotein purification. The method, requiring only simple process steps, affords full recovery of a target glycoprotein, and is effective at a low target glycoprotein concentration in the presence of large amounts of contaminants. This technique was then applied to the industrial application of soybean peroxidase purification, illustrating its targeting capacity in crude, natural protein extracts.
Optimized Insertion and Dissolution of Microneedle Patches in Human Subjects

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Vaccines are one of the most effective ways to reduce mortality associated with diseases and mostly delivered using needle and syringe. It requires trained personnel, creates medical sharps waste and requires cold chain. Dissolving microneedle patches contain micron-sized needles made of water-soluble biodegradable polymers that dissolve in the skin to deliver the vaccine. They offer the simplicity of patch application and the possibility to mitigate the challenges associated with hypodermic needles.
Saccharomyces cerevisiae: Designing Orthogonal Sensing Systems

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Escherichia coli and Saccharomyces cerevisiae (yeast) are the two major chemical production bio-machines used today in the biotech industry. Though yeast has a number of advantages over E. coli in industrial production, one of the major drawbacks in yeast-based production systems is a dearth of inducible promoters. To overcome this obstacle, we plan to exploit the yeast mating pathway, which is normally induced by pheromones secreted by yeast cells, leading to downstream expression of various genes like FIG1. We have engineered a yeast strain expressing a heterologous human olfactory receptor gene (OR1G1) that binds to a small molecule activators like nonanal leading to the expression of a reporter gene (GFP) under the promoter pFIG1. We also demonstrate that one yeast cell can selectively respond to multiple activators via multiple orthogonal receptors, which can be exploited for designing synthetic genetic circuits.
High-throughput Characterization of Morphological Phenotypes for Automatic Screening of *C. elegans* using Granulometry and Microfluidics

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A major challenge in image processing is the characterization of densely packed overlapping objects. Segmentation algorithms have been used for object recognition; however, development of an appropriate algorithm for a high degree of occluded objects is difficult. To solve this issue, we present an algorithm for semi-quantitative textural analysis of biological samples using the principles of granulometry. We demonstrate the capability of this algorithm by conducting an automated high-throughput screen of lipid droplet size distribution phenotypes in *C. elegans*. Coupling the algorithm with microfluidics allowed for the identification of new lipid storage mutants at approximately 500 times faster than previously capable. Ultimately, this algorithm can be used for identification of lipid droplet phenotypes in other organisms, and determining genes that disrupt lipid storage in *C. elegans* can broaden future investigations that will impact the genetic understanding of metabolism and fat storage.
A Route for Overcoming Strand Inhibition: Using Viscous Environments to Influence Nucleic Acid Kinetics

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An open question in understanding the chemical origins of life is how a proto-informational polymer—the precursor to DNA—replicated itself before the evolution of proteins. In the absence of enzymes, replication may have been driven by changes in environmental conditions, such as temperature. However, though a nucleic acid duplex can be thermally de-annealed into single strands, strand inhibition is a problem—duplex formation is so favorable that when the temperature is lowered, the single strands re-anneal before they can serve as templates for replication. Here, DNA is used as a model biopolymer to demonstrate that strand inhibition can be circumvented using viscous solvents, which destabilize duplex formation and kinetically trap DNA in a size-dependent manner. These solvents are attractive not only as a prebiotically feasible environment for enzyme-free replication but also more generally as a route for kinetically controlling nucleic acid binding and strand displacement events.
Architectural and Mechanical Cues Direct Mesenchymal Stem Cell Function on Cross-Linked Gelatin Scaffolds

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Naturally-derived biomaterials have emerged as modulators of cell function and tissue substitutes. Here, we developed cross-linked gelatin scaffolds for the expansion and osteogenic differentiation of mesenchymal stem cells (MSCs). The mechanical and architectural properties of the scaffolds were altered by varying the concentration of gelatin and glutaraldehyde, which ultimately determined the differentiation potential of MSCs cultured on the scaffold. ALP activity (osteogenic marker) of differentiated MSCs on higher gelatin concentration scaffolds was dependent on traditional effectors, including matrix elasticity and cell spread area. In contrast, the differentiation capacity of cells cultured on lower gelatin concentration scaffolds did not correlate with these factors, instead were dependent on the hydrated pore structure. These results suggest scaffold composition can determine what factors direct differentiation and may have critical implications for biomaterial design.
Microneedle Patches for Point-of-Care Diagnostics

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Microneedles are microscopic needles that can access dermal interstitial fluid bypassing the stratum corneum in a reliable, pain-free and easy-to-use manner, making them ideal for use as a diagnostic or monitoring system. They do so by bypassing the stratum corneum, and acting as conduits for transport of fluid into a central backing layer. Thus, microneedle patches can be developed into simple point-of-care diagnostic tests that would otherwise require expertise of collecting painful blood samples and clinical testing. Flexibility with materials and techniques for fabrication of microneedles allows us to engineer and fabricate various microneedle patch designs that exploit different materials and driving forces to draw fluid from the skin into the needles. The fluid can be eluted out to analyze for concentration and presence of desired biomarker. We have validated fluid extraction in pig cadaver skin. We are optimizing microneedle patches to minimize extraction time and maximize volume.
Effects of NO$_x$ on the Volatility of Secondary Organic Aerosol from Isoprene Photooxidation

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The effects of NO$_x$ on the volatility of the secondary organic aerosol (SOA) formed from isoprene photooxidation are investigated in environmental chamber experiments. Two types of experiments are performed. In HO$_2$-dominant experiments, organic peroxy radicals (RO$_2$) primarily react with HO$_2$. In mixed experiments, RO$_2$ reacts through multiple pathways, including with NO, NO$_2$, and HO$_2$. The volatility and oxidation state of isoprene SOA are sensitive to and exhibit a non-linear dependence on NO$_x$ levels. Depending on the NO$_x$ levels, the SOA formed in mixed experiments can be of similar or lower volatility compared to that formed in HO$_2$-dominant experiments. The dependence of SOA yield, volatility, and oxidation state on NO$_x$ level likely arises from gas-phase RO$_2$ chemistry and succeeding particle-phase oligomerization reactions.