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.
Microelectrodes for High-Power Energy Storage Devices

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With the widespread and shrinking size of portable electronic devices, there is a growing need for similarly scaled energy storage systems. These systems are expected to have the capability of rapid charge and discharge rates with a minimum loss in energy storage. Conventional batteries possess high energy density enabling them to supply energy for long periods of time, yet often lack similarly high power density. Supercapacitors, on the other hand, are capable of very fast charge and discharge rates due to their extremely high power density; however, the amount of energy they can store is quite limited compared to batteries. Our research focuses on the utilization of MEMS technologies to fabricate well ordered, high-surface area, three dimensional electrodes that are capable of carrying significant amount of currents to electrochemically active structures to bridge the application gap between these two energy storage mechanisms.
Controllable assembly of aromatic molecules on a surface via Diels-Alder reaction: A carbon source for graphene.

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ABSTRACT: Graphene is of tremendous interest based on its electronic properties, such as mobilities ≥ 200,000 cm²/V-s, as well as a very high thermal conductivity. Furthermore, graphene is one atom thick, making it a perfect substitute for silicon in small high performance devices. Graphene formation by directed chemical synthesis, utilizing intelligently designed precursors that can be converted thermally or chemically to graphene and graphene nanostructures with interesting electronic properties are of great interest. We successfully synthesized a silyl derivative of a maleimide that allows: (1) self-assembly to produce a controllable aromatic monolayer on a CMOS compatible surface, and (2) the ability to perform a reverse Diels-Alder reaction that allows us to obtain the carbonaceous starting material of interest in the surface for further thermal or chemical consolidation. Graphene so produced was analyzed and identified by Raman spectroscopy and other methods.
Carbon Molecular Sieve (CMS) membranes show enhanced gas separation capabilities. For industrial application of CMS membranes, it’s important to achieve this high performance in hollow fiber membrane configuration. The reason for the preference of this geometry is the asymmetric morphology consisting of porous support which leads to a high transport flux. During the preparation of CMS hollow fiber membranes, the thermal transition process collapses the porous support of polymer precursor which results in a drop in the transport flux. This process is known as Substructure Collapse.

In our study, we prevent the collapse in CMS hollow fibers by a process called as V-Treatment, which I’ll discuss in detail during my oral presentation. The enhanced CMS hollow fiber morphology after V-treatment shows an increase in gas separation productivity. In my poster, I’ll demonstrate the effect of V-treatment on CMS hollow fiber morphology and productivity from two different polyimide precursors i.e. Matrimid® and 6FDA:BPDA-DAM.
Impact of Functional Groups on the Topology and the Adsorption Properties of MOFs

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Metal-organic frameworks are a new fascinating class of nanoporous materials consisting of Inorganic ions or clusters coordinated to organic ligands to generate robust and often porous materials. The major advantage of MOFs over other traditional materials, such as zeolites or activated carbons, is their chemically-tunable structures with which MOFs are ideally suited for adsorption of gases and separation of gas mixtures. In order to optimize MOFs for more specialized applications, reticular synthesis approach has been used to modify the pore size and functionality of MOFs, which require the prerequisite that the functional groups do not interfere with MOF synthesis or alter the topology of the desired MOFs. However, in some cases the functional groups have strong effect on the topology of the parent MOFs, especially for the tricarboxylate ligands. HKUST-1 has been studied intensively and is one of a few commercialized MOFs. Our present goals are to assess how functionalization of ligands independently contributes to change or preservation of the HKUST-1 topology and to determine how functional groups affect the adsorption properties of MOFs.
A thermodenuder (TD) is an instrument that exposes a stream of particles to a known temperature profile for a given amount of time. Based on the volatilized amount of mass, characterized by the decrease in particle size, unique insights on the volatility of aerosol particles can be determined. Combined with an instrument that measures cloud condensation nuclei (CCN), particles that are able to become cloud droplets, further information of chemical transformations and hygroscopicity can be unveiled.

This project presents the design and testing of a TD paired with a comprehensive numerical model of aerosol flow through the instrument using size-selected (60-140 nm) aerosol composed of atmospherically-relevant compounds at a variety of temperatures (45, 55, and 65°C). This instrument is further used to probe particle evolution during toluene photo-oxidation, showing the potential for gas-phase surfactants rather than bulk particle chemistry alone to change the ability of particles to act as CCN.
Hydrogen is an important energy source for the future. One of the most important processes in producing high purity hydrogen is separating hydrogen from a mixture of gas streams. Membrane technology holds the key to the future of hydrogen production. This work looks at intermetallics; stoichiometric compounds of two or more metals as prospective membranes for these applications. Intermetallics are known to exhibit interesting structural and physical properties, which are often different from their constituents. We present a systematic computational screening approach based on calculation of key properties like solubility, diffusivity and permeability of hydrogen through these materials. Our calculations provide a useful method for analyzing a large set of materials and shortlisting materials that show properties useful for particular applications. We also employ the QSAR approach to develop a statistical model for the prediction of hydrogen binding energy as a tool based on fundamental properties of the elements.
PS-b-PAA and PS-b-PHEMA as High $\chi$ Polymers for Directed Self-Assembly

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As the semiconductor industry moves to smaller and denser IC manufacturing, directed self-assembly (DSA) of block copolymers has been shown to be a promising alternative lithographic process for production of sub-30nm pitch structures. PS-b-PMMA has been widely studied to self-assemble into large areas of regular grating structures with low defectivity. But PS-b-PMMA has reached its patterning limit approaching 20 nm using DSA, due to the modest $\chi$ value for PS-b-PMMA (0.038). We are investigating PS-b-PAA and PS-b-PHEMA as hydrogen-bond containing block copolymer materials with high $\chi$ value for sub-20 nm pitch patterning. Both of thermal and solvent annealings are used to mobilize these polymers to facilitate the self-assembly. The effects of these annealing methods were evaluated. While PS-b-PAA suffers from poor phase separation due to thermal cross-linking, PS-b-PHEMA shows better fit to industrial processing: the thermal stability is suitable for a thermal annealing without decomposition.
Current and future electronic devices and integrated circuits require metal interconnect films with low electrical resistivity and good resistance to electromigration-related failures. Metal layers are also of interest for plasmonic devices where distinct and tunable optical properties of metal nanostructures due to surface Plasmon resonance effects are needed. These applications demand that metal film dimensions and shapes be controlled to sizes below 100 nm. In order to achieve such structures, we are investigating the use of H$_2$-based plasmas to etch Cu, Ag, and Au. The exact etch mechanisms for these metals are somewhat different because of different bond strengths, atomic masses, and thermodynamic stability of etch products. However, chemical reaction between the metals and H radicals, whose rate appears to be enhanced by physical ion and photon bombardment, plays an important role in the etch processes for Cu, Ag, and Au.
Interactions of Biomass Molecules with Heterogeneous Catalysts in Aqueous and Vacuum Environments

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Aqueous phase catalytic processes for biomass conversion are promising because many biomass-derived compounds are soluble in water and because water is an abundant and environmentally friendly solvent. The current study investigates the fundamental interactions of biomass derived oxygenates with catalysts and supports. Specifically, the interactions of ethylene glycol, 1,2-propanediol, 1,3-propanediol, glycerol, with γ-Al₂O₃, TiO₂ anatase, ZrO₂, MgO and 5 wt% Pt on γ-Al₂O₃ were studied.

Transmission IR was used to investigate surface interactions between the various biomass derived oxygenates and the metal oxides. This analysis showed interactions with specific surface hydroxyls and alkoxide bond formation on Lewis acid sites as a function of co-adsorbed water.

Reforming kinetics of glycerol solutions over a 5 wt% Pt on γ-Al₂O₃ catalyst were studied using a flow ATR-IR setup. This study showed that the formation kinetics of hydrogen and carbon monoxide on the Pt surface is dependent on the catalyst layer pretreatment used.
Degradation Studies of Aminosilica Adsorbents for CO₂ Capture
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CO₂ capture and concentration from flue gases has become a widely researched approach to reducing anthropogenic CO₂ emissions. Amine oxide materials have emerged as a promising candidate for this process as they can possess high adsorption capacities, good adsorption kinetics and stability under humid conditions. Critical areas to explore for improvement in the design of these adsorbents relate to the degradation of these materials from thermal, oxidative of urea forming deactivation. In an effort to understand how the chemical structure of amine adsorbents affects the deactivation of these materials, a combined experimental and modeling study of the stability of various silane based amine materials was performed to evaluate structural properties that yield some materials’ enhanced stability. We demonstrate that there are differences in the performance of these materials as a function of amine type, which has significant implications for the rational design of aminosilica adsorbents for CO₂ capture processes.
Biopolymer Translocation through Solid-State Nanopore Devices: A Langevin Dynamics Study

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Small nanopores (1 – 10 nm diameter) constructed in solid-state membranes have shown promise as next-generation biopolymer analysis devices offering both high resolution and throughput. In this work, we use Langevin Dynamics simulations to investigate the translocation of DNA-like biopolymers through nanopores as a function of the nanopore dimensions, driving voltage, and biopolymer length for polymer models that include (Zimm) and omit (Rouse) hydrodynamic interactions. Based upon the simulation results, we elucidate the scaling laws of the translocation time of both “long” and “short” biopolymers as a function of their length and of the applied voltage. We discuss the physical implications of these scaling laws and their relationship to theoretical models and experimental data. This information can be used in designing algorithms for operating nanopore devices and to interpret the experimental data more reliably.
Enantiomers are important building blocks in the manufacture of multiple pharmaceutical compounds such as anti-inflammatory agents, antibiotics, pain relievers, and gastrointestinal drugs. Chiral chromatography and classical resolution are commonly used to purify racemic mixtures. However, such processes involve the addition of organic solvents or strong acids/bases. Also, the isolation of the desired enantiomer can involve multiple steps. As a result, the overall efficacy of the process is reduced. Due to the constant increase of the enantiopure drugs market, processes of higher efficiency are of great interest. Toward this end, we are designing a reactive-crystallization based process in which enantiomerically pure crystals are recovered from a reactive solution. The process consists of development of ternary phase diagrams to identify zones in which enantiomerically pure compounds can be recovered through crystallization. Later, enantioselective enzymatic reactions are performed in supersaturated solutions to maintain the concentration within the desired region. The process was proven by performing the chemo-enzymatic stereoinversion of DL-phenylalanine by D-amino acid oxidase (D-AAO) under supersaturated conditions. By performing such a reactive separation, we were able to maximize the rate of reaction, and obtained crystals with a chemical and enantiomeric purity greater than 99%. Finally, the process has been extended to multiple reactions and a continuous operation is being developed.
Mesenchymal stem cell (MSC) recruitment from bone-marrow (BM) is a critical step for in vivo tissue regeneration. MSCs undergo migration and subsequent tissue-specific differentiation under the influence of soluble factors. Though the molecular responses of MSCs to soluble factors have been studied extensively, the mechanical properties that govern their response are yet to be fully understood. We sought to investigate effects of soluble factors, transforming growth factor-β1 (TGF-β1) and platelet-derived growth factor (PDGF-BB), on MSCs mechanics. Treatment with the soluble factors for 24 hours dramatically altered the morphology, cytoskeletal organization, intracellular rheology and adhesivity of MSCs. TGF-β1 treated MSCs required synergistic activation of PDGF-BB signaling to induce mechanical stiffening. A genome-wide microarray analysis revealed regulation of genes involving cell migration, actin cytoskeleton, extra-cellular matrix remodeling, cell cycle and development.
Recursive Dynamic Framework using Multivariate Gaussian Process Models for Stochastic Simulations

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Gaussian process models (GPM) have been implemented with great success in the area of dynamic systems modeling for its flexibility and accurate results. However, most of these applications only consider the prediction of a single output variable for control or state estimation. Here we present a comparison between two mathematical frameworks for the predictions of a multivariate stochastic system dynamics based on GPM. We compared a framework that builds an independent GPM (iGPM) for each of the predicted state variables, and a framework that simultaneously generate a multivariate GPM prediction (mGPM), using an additional covariance function to describe the correlation of output samples. Despite that mGPM exhibits an improvement in the mean prediction error of approximately 6% compared to the iGPM, this last mathematical framework is recommended for future applications of Gaussian process models in the area of systems dynamics, due to its simplicity of implementation and similar performance.
Elucidating Chemical Stability and Proton Conductivity of Proton Conductors through First Principles Modeling

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A longstanding aim in development of electrolytes has been to find dopants that give high proton conductivity coupled with good chemical stability. Perovskite-type oxides are useful materials for proton conduction. We used first-principles calculations to address this topic in doped BaZrO$_3$ with efficient methods to examine a wide range of possible dopants (Y, In, Ga, Sc, Nd, Al, Tl, Sm, Dy, La, Pm, Er, and Ho). These calculations correctly identify the doped BaZrO$_3$ materials that are already known to have favorable properties, but also identify a number of materials that have not been examined previously as promising. We investigated the physical origins of the trends in chemical stability and proton mobility among different dopants. Our data allow us to consider several possible physical descriptors for characterizing doped perovskites as proton conductors.
The quality of products in particulate processes highly depends on the particle size distribution, which is developed by mass-transfer at interface boundary. Therefore, to monitor and control the processes, understanding the kinetics of both particles and the liquid phase is important.

In this work, we used focus beam reflectance measurement (FBRM) to measure the crystal size distribution (CSD) and ATR-FTIR for solute concentration, both in situ and online, in a paracetamol-ethanol batch cooling crystallization system. A linear model of the FBRM has been constructed and validated by our experimental results. Simultaneously the IR spectrum was utilized to estimate the solute concentration. With a tailored optimization algorithm, the CSD was estimated to visualize the dominating crystallization kinetic events occurring at different operating conditions. Our approach greatly enhances the capability of the FBRM and reveals its potential in kinetic parameter estimation and real-time control of particulate processes.
Aminosilane-Functionalized Hollow Fiber Sorbents for Post-Combustion CO₂ Capture

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Carbon dioxide, a main by-product of fossil fuel combustion processes, has become a major environmental concern due to the gradual increase of its global atmospheric concentration in recent decades. The capture of CO₂ from coal-fired power plants is critical for mitigating greenhouse emissions. In this study, porous polymeric hollow fiber sorbents with fast sorption kinetics and improved sorption capacities were prepared by functionalizing aminosilane to cellulose acetate hollow fibers as a “proof of concept”. A lumen-side barrier layer was also developed in the aminosilane-functionalized cellulose acetate fiber sorbent to allow for facile heat exchange without significant mass transfer with the bore-side heat transfer fluid. Lumen layer formation allows the real application of hollow fiber sorbent into rapid temperature swing sorption process. The functionalized cellulose acetate fiber sorbents were characterized by pressure decay sorption measurements, multi-component column chromatography, FT-IR, elemental analysis, and scanning electron microscopy.
The concentration of CO₂ in the atmosphere is increasing at an accelerating rate from decade to decade and it has caused a series of problems. Coal-fired power plant is a major source for atmospheric CO₂. Many methods have been developed to reduce CO₂ emissions from coal-fired power plants. In this work, polymeric membranes are used to capture CO₂. Due to the highly condensable property of CO₂, it behaves abnormally at sub-ambient temperatures, making the separation of CO₂ from flue gas easier. Asymmetric hollow fiber membranes with fused nodular selective layers have been successfully spun. With silicone rubber (PDMS) caulking, this kind of hollow fibers displayed both high CO₂/N₂ selectivity and high CO₂ permeance at sub-ambient temperatures. A hypothesis regarding the introduction of Langmuir sorption sites is proposed to explain the good performance of the caulked nodular-skinned fibers.
Designing changes in phase equilibria enables the facile and efficient recovery of homogeneous catalysts and their subsequent recycle. Organic-Aqueous Tunable Solvents (OATS) can be used to couple homogeneous reactions (fast rates and high selectivity) with heterogeneous separations. Upon reaction completion, the separation is simply conducted by applying CO$_2$ pressure to manipulate the phase behavior of the initial monophasic organic–water mixtures. As a result, a phase split can be induced resulting in two phases: one organic-rich and one aqueous-rich phase. The products are separated at this stage (organic-rich phase) from the catalysts-containing phase which can now be recycled. Few examples will be presented and discussed, including the Rhodium-catalyzed hydroformylation of model compounds applicable to the synthesis of ibuprofen. We will demonstrate that very modest CO$_2$ pressures (3-4 MPa) enable the recovery of up to 99% of the product and 99.9% of the relatively hydrophobic catalyst. The presentation will be aimed at demonstrating the breath of OATS technology to develop alternative strategies toward the sustainable production of pharmaceuticals.
Catalytic Upgrading of Pyrolysis Oil Derived from Lignin

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Lignin, as the 2nd most abundant component in lignocellulosic biomass, remained intact during the bio-ethanol production and usually was burnt directly. In my research, pyrolysis oil derived from lignin was upgraded with several noble metal catalysts. Five-factor ANOVA was done to study the effects of the reaction condition. The major two compositions of pyrolysis products, light oil and heavy oil, were upgraded separately. Fully hydrogenated and intensively deoxygenated products were obtained from both compositions. Advanced NMR technique and GC-MS were used to identify the feeding materials and final products. To understand the reaction mechanism and difference between catalysts, various model compounds were used. The deactivation of catalysts was observed in the upgrading process and the mechanism was studied. Finally the optimization of the pore structure and acidity was done to increase the selectivity and the yield in the upgrading process.
Rational Engineering of Nanowire Superstructures

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Semiconductor nanowire synthesis provides a promising route to engineer novel nanoscale materials for applications in energy conversion, electronics, and photonics. In order to enable the appropriate function for a particular application, control of atomic and nanoscale structural details (e.g. diameter, orientation, faceting) is critical. We demonstrate the ability to engineer nanowire structure by tuning chemistry either at the nucleation point or on the sidewall, thus enabling the rational fabrication of complex superstructures for the first time. Specifically, we have gained the chemical understanding necessary to select crystal growth direction and create kinking superstructures with well-defined angles and segment lengths. Additionally, we demonstrate user-programmable diameter modulation using permanent or temporary surface chemistry motifs, decoupling of axial and radial growth kinetics via catalyst alloying, and combinations of these strategies to create complex nanoarchitectures. These new synthetic strategies comprise a much needed toolbox for the precision engineering of nanoscale structures and materials properties.
A Detailed Study of High-Pressure Biomass Pyrolysis in an Entrained-Flow Reactor

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A major advantage of biomass gasification is that any lignocellulosic material can be converted to syngas and subsequently to bio-fuels. In a gasifier, pyrolysis and char gasification steps are known to occur in series. Thus it becomes important to study the characteristics of pyrolysis products such as chars, gases and tars, since these have an effect on the char gasification kinetics. In this work, pyrolysis of pine and switch grass was performed in an entrained flow reactor at high temperatures (600-1000 °C) and high pressures (1-20 bar). Heating rates as high as 104 K/s were achieved with solids residence time from 3-20 s. Analytical techniques such as SEM and N2 Physisorption, micro-GC and GC-MS were used to analyze the pyrolysis chars, gases and tars respectively as a function of pyrolysis variables. The present study will provide a basis for improved understanding of the biomass pyrolysis and lead to mathematical modeling of char gasification based on meaningful descriptors.
Computational Methods to Identify Metal Hydrides for High Temperature Tritium Sequestration

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The DOE’s Next Generation Nuclear Plant demonstration project will use a very high temperature reactor with helium coolant outlet temperatures between 1000 and 1200 K. To avoid quenching the industrially-useful process heat, we are applying first principles methods to identify metal hydrides capable of removing the dilute tritium contaminant from the coolant. We establish the minimum level of theory (i.e., harmonic, thermal expansion, etc.) needed to describe the thermodynamics of metal hydride systems at high temperature and investigate the effect of hydrogen isotope substitution. Then, since ternary hydride systems (two metals) are typically metastable to the associated binary (pure metal) hydrides, we use a grand potential minimization technique to confirm conditions under which the anomalous Th-Zr-H ternary interstitial hydride may be thermodynamically more stable than the associated binary hydrides as a proof of principle calculation.
Simulation of Diblock Copolymer Directed Self Assembly Processes: Applications for Semiconductor Manufacturing

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Traditional photolithography has been used to shrink transistor size and increase semiconductor manufacturing capability for over fifty years. However, traditional methods are beginning to hit their limits as transistor size continues to shrink. One way in which this can be attacked is via a bottom up approach, namely directed self-assembly (DSA). DSA using block copolymers (BCP) is being considered as a supplement to traditional lithographic methods to continue to shrink transistor size in the coming years because of its natural tendency to phase separate into microdomains that are of useful size for the integrated circuit manufacturing industry. Simulation has the advantage of being able to produce results much more quickly than experiment, and so it is well suited to guide experimentation and to produce design rules for semiconductor manufacturing. Here I describe and use a coarse grained molecular dynamics model for BCPs that will be used to prescribe such design rules base on various parameters of importance including pitch, line roughness, and defectivity.
Intracellular Drug Delivery Through Photo-acoustic Generation of Laser Particle Interaction

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The hypothesis that laser can be preferentially absorbed by a nanoparticle solution, which can in turn lead to generation of photo-acoustic waves leading to cell membrane poration, was tested. A Nd:YAG nanosecond laser was used to shine a solution of carbon, uptake marker and cells. The uptake and death was quantified using a flow cytometer. Under the conditions tested, at 100mJ/shot a maximum of 70% of live cells uptake with >90% viability was observed. A stronger effect of laser was observed when the energy output of the laser as well as the time of exposure was increased. The presence of photoacoustic waves was determined by using a hydrophone. The temperature change in the solution was measured using an IR camera.
Surface Hydrogen Stabilized Semiconductor Nanowire Growth

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Semiconductor nanowires exhibit unique optoelectronic properties that are attractive for energy conversion, electronics, and photonics. While previous reports demonstrate nanowires with complex structures, the inability to rationally manipulate their synthesis limits the design space. To advance structural diversity, fundamental knowledge of the chemical bonding that governs nanowire growth is required. To that end, we studied the role of hydrogen during germanium nanowire synthesis with real-time in situ infrared spectroscopy. We show that surface hydrogen is coincident with stable \( <111> \) germanium nanowire growth and influences sidewall taper. To demonstrate this behavior, we synthesized uniform arrays of \( <111> \) germanium nanowires via a two-step growth process followed by elongation at various process conditions. Infrared spectroscopy is used to monitor the evolution of chemisorbed hydrogen on the nanowire (1990 – 1960 cm\(^{-1}\)) during its growth. We specifically observe absorption bands, at 1980 cm\(^{-1}\) and 1965 cm\(^{-1}\), that are coincident with stable nanowire growth.
Nucleation Study on Dendrite Suppressing Lithium-Sodium Electrolyte for Lithium Batteries

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High energy density batteries are desired for smaller, lighter mobile devices. A lithium metal anode is an intriguing possibility because it represents the maximum achievable energy density for a lithium-based battery, 3861 mAh/g instead of 329 mAh/g for commercial graphite anodes. A major deterrent is that lithium metal electrodeposits into long whiskers that can short circuit the battery. We used a lithium-sodium codeposition to mitigate this dendrite growth. Lithium dendrites likely grow due to certain crystal faces being more electrochemically active than others. Sodium may deposit preferentially on these sites, resulting in a dimpled morphology that blocks dendrite growth. A detailed study on the nucleation and early morphology has been completed. Analysis of current-time transients showed significant deviations from conventional models due to the effect of the solid electrolyte interface (SEI) layer. The model was adapted to better explain the behavior observed from electrochemical and SEM data.
Geometric Characterization of the Fontan Connection and its Relationship with Hemodynamic Outcomes

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The Fontan procedure is applied to sustain life in patients born with single ventricle heart defects. It involves connecting the vena cavae to the pulmonary arteries to bypass the malfunctioning ventricle. As these patients grow, various complications develop, which may be attributed to the unfavorable connection hemodynamics. The Fontan anatomies are complex and their geometric characteristics can impact the hemodynamic outcomes. This study was carried out to understand how the anatomic features correlate with the hemodynamic outcomes. 100 patient-specific 3D anatomies and flow waveforms were reconstructed from cardiac magnetic resonance images. Geometric features were extracted and blood flow characteristics were simulated using computational fluid dynamics. It was found that vessel diameter, distance between the vena cavae and angles across the connection were strongly correlated to hemodynamic outcomes. Such information can be important for future surgical designs to improve patient outcomes.
Evaluation and Application of New Nanoporous Materials for Acid Gas Separations

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Natural gas separations and purification are currently operated by resource intensive processes, such as liquid amine absorption to remove acid gases from product streams. Nanoporous materials offer a unique, low-energy alternative to traditional separations by utilizing either adsorption- or membrane-based technologies. Zeolitic imidazolate frameworks, a subclass of metal-organic frameworks, are shown to have tunable separation properties by using a novel mixed-linker approach. Both the adsorption and transport properties of these ZIFs materials are presented to show changes in separation performance depending on either the linker composition and/or the processing conditions. Overall, the adsorption studies show that mixed-linker ZIF materials offer improvement for CO₂/CH₄ separations over commercially-available adsorbents. Using composite, or “mixed-matrix”, membranes, ZIF materials dispersed in commercial polyimide membranes show CO₂/CH₄ separation enhancement over the pure polymer membrane, indicating defect-free membrane formation and a promising route for acid gas or other molecular separations.
While it has been known for almost a century that energy metabolism in cancer cells is dysfunctional, only recently has the importance of metabolism in cancer come to be more generally recognized. Despite some targeted study of metabolism in cancer, its systems-level dynamics remain unexplored. A deeper understanding of these metabolic behaviors could profoundly affect the way that cancer is understood or even treated. To explore the systems-level dynamics of cancer metabolism, the dynamic responses of epithelial ovarian cancer cells to perturbations \textit{in vitro} are profiled. The perturbations reflect biological stresses that normally occur in cancer, such as nutrient deprivation and hypoxia. The perturbation experiments are performed over a time span of multiple days. Extracellular and intracellular samples are taken and then processed and analyzed using 2D gas chromatography coupled to mass spectrometry. The results of these experiments will determine the metabolites that are altered by the biological perturbations.
Particle stabilized emulsion, also known as Pickering emulsions, have attracted recent attention as versatile alternatives to classical, surfactant-stabilized emulsions, and as a basis for microencapsulation schemes. The present study investigates two widely overlooked effects of electric particle charge on the particles’ ability to adsorb to emulsion droplets and stabilize them against coalescence: the so-called image charge interaction between particles and a nearby liquid interface, and the influence of electrostatic fields on the equilibrium position of interfacially adsorbed particles. Taking these effects into account, we can explain qualitative discrepancies between emulsification experiments and the most widely adopted theoretical predictions. The obtained insights are used, in a more applied portion of our work, to aid the design of emulsion-templated microcapsules for sustained and controlled release of active cargoes, for instance in the antimicrobial functionalization of paper and packaging materials.
We will present numerical and experimental studies of depletion-induced interactions between hard colloidal particles and structured surfaces. The objective of our work is to show that selective self-assembly of colloids onto hard substrates can be achieved by controlling surface geometry. A generalized numerical model was developed for calculating the interaction potentials between hard spheres and surfaces with increasing geometrical complexity in order to assess the feasibility of experiments a priori and guide the design of new surface geometries. The experimental work was used to benchmark the model: a phase diagram of the different modes of adsorption was created for colloid/polymer solutions on flat and structured substrates as a function of polymer and salt concentrations. The experiments showed that selective adsorption of colloids can indeed be achieved. Future work will focus on more complex three-dimensional structures and use of other depletion-inducing agents.
Resist Surface Crosslinking Using Multifunctional Amines to Mitigate Pattern Collapse in Thin Film Lithography

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As the semiconductor industry continues to push to smaller critical dimensions, pattern collapse caused by unbalanced capillary forces during the final rinse and drying process has become an important problem that can practically limit the resolution of a resist material long before its intrinsic resolution limit is reached. The main forces which govern such pattern deformation are related to mechanical properties of the resist. Instead of synthesizing and changing the chemical formula of the resist, the quick way for achieving the mechanical enhancement is to crosslink the resist surface using surface reactive rinse. In this work, the use of multi-functional amines to reactively crosslink the surface of resist containing carboxylic groups through formation of amide bonds using carbodiimide chemistry has been explored. Contact angle studies and X-ray photoelectron spectroscopy (XPS) were used to characterize the surface crosslinking reaction after surface rinse treatment. Pattern collapse test structures were fabricated and analyzed to quantify the impact of the use of amine reactive rinse treatment. XPS spectra, SEM images, and critical stress analysis of the resulting patterns confirmed that the use of reactive rinse can significantly enhance the mechanical properties of the resist and dramatically mitigate pattern collapse.
Olefins are consumed as feedstocks to produce a variety of significant chemicals. Membrane separation is an energy-efficient alternative to distillation, which is traditionally used to separate light olefins from co-products of steam crackers. Mixed-matrix membranes formed by dispersing molecular sieve (e.g. zeolites, CMS, and ZIFs) particles in polymer matrices combine the ease of processing polymers with the superior separation performance of molecular sieves. Our previous studies on adsorption kinetics suggested that ZIF-8 was remarkably size/shape selective for C₃ and C₄ hydrocarbons. We also demonstrated that ZIF-8 was capable of enhancing C₃H₆/C₃H₈ separation performance in the matrix of polyimide 6FDA-DAM. In this study, efforts were made to scale up the successful platform of ZIF-8/6FDA-DAM mixed-matrix dense films to an industrially practical form, i.e. asymmetric hollow fiber membranes through dry-jet/wet-quench spinning. Microstructure of the dual-layer mixed-matrix hollow fibers was characterized and C₃H₆/C₃H₈ separation performance was evaluated by gas permeation tests.