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SECTION A: NEW SYNTHESIS METHODS

(1) RAPID SYNTHESIS OF FUNCTIONALIZED DENDRONS THROUGH CLICK CHEMISTRY
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The divergent growth of aliphatic ester dendrons based upon 2,2-bis(hydroxymethyl)propionic acid (bis-MPA) has been accomplished in high yield by the use of the anhydride/DCC coupling steps. Monodisperse, fourth generation dendrons were synthesized using mild reaction conditions which allowed azide and acetylene functionalities to be easily introduced at the focal point of the dendrimers. The presence of the azide and acetylene groups permitted Click Chemistry to be used for the functionalization of the dendrons. The facile nature of Click Chemistry allows a wide range of different focal point groups to be introduced and permitted the coupling of the dendrons to produce novel functionalized, asymmetric dendrimers.

(2) NEW FUNCTIONAL OLIGOMERS AND POLYMERS USING N-HETEROCYCLE CARBENE AND CLICK CHEMISTRY
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Hydrogels are a type of biocompatible polymer, and are being used in the development of a synthetic cornea and synthetic corneal onlay. We are looking to prepare a series of networks with controlled architecture, resulting in new, tougher hydrogel materials. We are currently exploring new ways to generate these hydrogels using click chemistry. Click chemistry has proven useful for this purpose due to the fact that it is a simple, highly selective reaction that can be performed under mild reaction conditions. In addition, we have been conducting research with N-heterocycle carbenes, which have been shown to be effective catalysts in the synthesis of polylactides. Polylactides are biocompatible and biodegradable polymers, and are ideal for a number of applications, including uses in the biomedical field, drug delivery, and as environmentally friendly packaging materials. We are currently exploring new strategies to synthesize functional lactides. In addition, we have also been able to show that N-heterocycle carbene catalysis is compatible with click chemistry, opening the door for any number of future functional lactide syntheses.
(3) MODULAR SYNTHESIS OF RAFT AGENTS VIA CLICK CHEMISTRY FOR THE PREPARATION OF VARIOUS WELL DEFINED CHAIN-END FUNCTIONALIZED POLYMER ARCHITECTURES

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We have developed a new synthetic approach combining reversible addition fragmentation chain transfer (RAFT) polymerization with “Click” chemistry for the preparation of well defined chain end functionalized polymer architectures. A series of novel RAFT transfer agents were synthesized via “Click” chemistry involving the coupling of organic and inorganic azides to acetylene derivatized RAFT transfer agents through the stereoselective formation of a 1,4-disubstituted 1,2,3-triazole ring. Utilizing these new functionalized chain transfer agents, organic and hybrid organic/inorganic architectures were synthesized from the RAFT mediated polymerization of styrene, methyl methacrylate, t-butyl acrylate, and N,N-dimethylacrylamide. The resulting chain end functionalized polymer architectures, i.e. linear and block copolymers, exhibited low polydispersity in the range of 10000 < Mn < 80000 g/mol and were characterized using nuclear magnetic resonance (1H and 13C) and size exclusion chromatography (SEC).

(4) EXPANDING THE SCOPE OF N-HETEROCYCLIC CARBENE CATALYSIS

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N-Heterocyclic carbenes have been shown to be effective catalysts in the metal-free synthesis of polyesters and polylactides. We seek to extend the functionality of nucleophilic carbene catalysts to the synthesis of polyester-ethers (poly p-dioxanone) and polypeptides. These biodegradable and biocompatible polymers are ideal materials for use in drug delivery, hydrogels and other medical applications. We further seek to prepare functionalized polyester-ethers that are amenable to modification via click chemistry.

(5) SYNTHESIS OF N-HETEROCYCLIC CARBENES: ORGANIC CATALYSTS FOR POLYMERIZATION AND ESTERIFICATION REACTIONS

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N-heterocyclic carbenes have worked well as organic catalysts for living polymerization of lactone and lactide. The ring-opening polymerization (ROP) via these carbenes provides molecular weight control and low polydispersity within the polymer product. We would like to extend the utility of these catalysts into the field of asymmetric transformations, which would give us still greater control over polymer properties. The chiral carbenes synthesized from 1R, 2R, 3R, 5S-isopinocampheylamine were studied to determine their stereoselective effect on racemic lactide and their possibility as esterification catalysts for chiral alcohols. Our research involving the synthesis of chiral n-heterocyclic carbenes and their use as ROP catalysts will be presented.
N-heterocyclic carbenes (NHCs) have shown great promise as organic catalysts for living polymerization of lactones and lactides. They offer precise control of molecular weight and low polydispersity without trace metal contamination in the final polymer product. However, since carbenes are extremely air and moisture sensitive, we are working to develop air-stable adducts of NHCs that can generate active carbene species \textit{in situ}. Of particular interest are adduct of NHCs and alcohols, which can undergo an elimination reaction to generate alcohol and free carbene. These adducts act as a combination catalyst/initiator for polymerization reactions, and are extremely active at room temperature. These NHC adducts give the same endgroup control as the free carbenes, and can be made from a variety of alcohols. Adduct mechanistic studies and polymerization data will also be presented.

Our interest focuses on low-k silicon type polymers that cross-link under thermal treatment. Si-H containing polycarbosilanes represent an interesting class of materials which meet this criterion. Unfortunately, cross-linking is only achieved when oxygen is present, whereas the target process should be working under a strictly inert atmosphere. Functionalization of polycarbosilanes with vinyl groups should allow thermal cross-linking under these conditions. Grafting of vinyl groups on the polycarbosilane was achieved via a hydrosilylation reaction using a divinyl derivative (DMDVS). When a homogeneous platinum catalyst (Speier catalyst – H\textsubscript{2}PtCl\textsubscript{6}\textsubscript{6H\textsubscript{2}O}) is used, while effective, a large amount of undesired metal is trapped in the polymer at the end of the reaction. In order to overcome this issue, heterogeneous Pt nanoclusters were used, leading to low platinum content, functionalized polymers which cross-link after treatment at 250°C for 2 minutes under N\textsubscript{2}.
SECTION B: NANOPOROUS MATERIALS

(8) SYNTHESIS OF AMPHIPHILIC NANOPARTICLES AS PORAGEN MATERIALS FOR LOW-K DIELECTRIC APPLICATIONS
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The need to shrink the size of computer chips has been limited by the dielectric properties of the materials available to prevent current leakage between wires. For this to be achieved, materials with dielectric constants of 2.0 or below must be developed. This can be achieved by spin coating low-k materials with appropriate poragens to create porous thin films which will have lower overall dielectric constant. The aim of this project is to synthesize amphiphilic nanoparticles as poragen materials to allow for the maximum amount of pores as well as mechanically strong films. These porogen materials were synthesized via a “core-out” scheme producing multi arm polystyrene star molecules by ATRP polymerization. The periphery of these polystyrene stars were further functionalized with polyethylene glycol using ethanol amine or diethanol amine bridges. The architecture of these molecules as well as their amphiphilic nature allows the nanoparticles to be completely compatible in the low dielectric matrix material and yet keeping the polystyrene cores isolated to generate discrete spherical and isolated pores.

(9) MECHANICAL AND FRACTURE BEHAVIOR OF NANOPOROUS THIN-FILM MATERIALS PRODUCED USING TEMPLATION-VITRIFICATION-THERMOLYSIS STRATEGIES
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From biological scaffolds to dielectric layers, nano-templated organic-inorganic hybrid glasses are being developed to yield a versatile class of highly porous materials with tunable properties. However, the mechanical properties, particularly adhesion and cracking behavior, of these low-density brittle glasses are expected to deteriorate with the incorporation of nanoporosity. In this study, we demonstrate remarkable toughening behavior in highly porous Methysilsesquioxane (MSSQ) films attributed to molecular bridging by molecular remnants of the pore-generating copolymer. Adhesion data at several selected interfaces is presented as a function of porosity for different porogen-matrix systems. Interfacial toughening was reported for nanocomposites in which the porogen did not totally volatize. This resulted in increasing adhesion energy at an MSSQ-SiO2 interface with increasing porosity. X-ray and infrared spectroscopy clearly show remnants of the porogen molecule at the interface. A molecular bridging model is used to explain increases in the adhesion energy of up to 1000%. Further mechanical tests with organic/inorganic hybrid films cured to various temperatures showed a preference to de-bond between the MSSQ films and the Si substrate. Adhesion properties were also found to be dependent on the curing temperature as the MSSQ matrix vitrified and the porogen volatized.
(10) REAL TIME BINDING KINETICS OF LIGAND PAIRS IN POROUS SILICA FILMS
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Biomolecular binding in porous silica films was studied in real time using surface plasmon resonance. The effects of porosity and film thickness on the binding kinetics of protein A-IgG were examined. The porosity and thickness of the films varied from 50%-65% and 300 nm - 500 nm, respectively. It has been proposed that the enhanced surface area provided by these films allows for a higher degree of molecular interactions. However, transport in and out of these films may be hindered by the tortuosity of the silica structure.

(11) STAR POLYMER TEMPLATED MESOPOROUS TITANIA FILMS FOR PHOTOVOLTAIC APPLICATIONS
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Silicon based photovoltaic cells are too costly to be used for widespread energy production. A new type of low cost photovoltaic cell can be made by patterning semiconducting polymers and inorganic semiconductors around each other at the nanometer length scale. Electron transfer occurs when excitations are split at an interface between the two semiconductors. The resulting current can be used to produce affordable solar energy. In this project, we have found a method for making star polymer templated mesoporous titania films and study the effect of processing conditions and polymer infiltration techniques on the efficiency of electron transfer in the films. We use ultra high resolution SEM and ellipsometry to characterize the films and make photoluminescence quenching and absorption measurements to study electron transfer. We show that titania films with a uniform distribution of pore sizes can be made using a star polymer as a structure-directing agent and that about 75% of the total volume of the film can be filled with semiconducting polymer. Our preliminary results are promising and the next step is to test the efficiency of a photovoltaic device.
SECTION C: MICROCONTACT PRINTING AND MOLDING

(12) NANO-IMPRINTING OF POROUS DIELECTRIC MATERIALS
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The current patterning process for BEOL integration makes up about 75% of the total wafer process cost. Therefore, a simpler and more effective method to create patterned porous films is highly desirable. Nano-imprinting provides an interesting approach to solving this problem. However, the first low dielectric material auditioned for this novel process, methyl silsesquioxane (MSSQ), is a solid that is difficult to imprint; a liquid material would be preferred. Oxycarbosilanes are liquid polymers that can be cross-linked by sol-gel processing using an acid or base catalyst. Thus, one possible approach involves the stamping of a liquid oxycarbosilane, a thermal acid generator (TAG), and solid MSSQ flakes dissolved in this solution in order to promote a cross-linking reaction. This solution is in the desirable liquid phase which is appropriate for applying a mold and imprinting processes. Current results show this process is capable of producing porous, low-k materials (k<2.2) that are suitable for imprinting.

(13) NOVEL TECHNIQUES FOR RAPID AND VERSATILE SURFACE MICROSTRUCTURE FORMATION
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Rapid prototyping techniques were investigated to create hydrophobic polymer surfaces with lateral structure dimensions in the sub-100 micrometer length scale. This was attempted using a laser printer, polyethylene terephthalate (PET) films as a medium, and various chemical surface modification techniques which include: O₂ plasma treatment, selective dissolution, silanization chemistry with distinct silanes, electroless metal deposition, and ion etching. A Hewlett Packard (HP) 2100TN laser jet printer, pushed to the limit of its resolution (1200 dpi), was employed to create an array of printed dots as a mask for selective modification of the PET transparency surface topography. Several approaches were investigated, and the most precise patterns were generated through direct printer manipulation using HP’s Printer Command Language (PCL) which resulted in ink-dots 80 μm in diameter. Surface attached perfluorodecyltrichlorosilane (FAS) groups provided very hydrophobic surfaces, with static contact angles approximately 130°± 5°. Electroless copper deposition and ion etching techniques are currently being studied to facilitate the formation of rough surfaces, which may add to the dewetting properties of the PET film.
(14) A SIMPLE AND GENERAL ROUTE FOR THE FABRICATION OF ELECTRONIC DEVICES BY MICROCONTACT PRINTING

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In this study, we demonstrate a method for fabricating electrodes by patterning gold substrates with an elastomeric stamp coated with organic self-assembled monolayers (SAMs). SAM molecules have sulfur-containing groups that are resistant to etchant solutions. Regions of the gold substrate that do not come into contact with the raised features of the stamp can then be etched away. The resulting gold electrode pattern may be used in electronic devices such as field-effect transistors or microelectrodes for sensor studies. A variety of different SAMs were tested as stamps to achieve optimum patterning specifications. In this study we show that “micro-contact printing” is an effective method for fabricating a wide range of electrodes with fine-tuned features and dimensions. This method can also be applied to platinum and silver electrodes.

(15) THIOL-ENE RESINS FOR NANOCONTACT MOLDING

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We have developed a nanocontact molding (NCM) process in which thiol-ene photopolymer resins are used. The NCM process has traditionally utilized meth/acrylate monomer mixtures which are photopolymerizable when exposed to 365 nm wavelength light. Thiol-ene mixtures are advantageous due to their lack of inhibition by oxygen. The main difficulty in using thiol-ene resins has been the adhesion of the polymeric mold to the photopolymer resin after curing. To overcome this problem, we worked to modify the surface chemistry of the mold. Treatments including oxidation, fluorination, and heating as well as soaking in water, acid, base, alcohols and other organic solvents were attempted. In the end we found that soaking the mold in chloroform for 2.5 hours allowed for optimal release properties. Through the utilization of stamps prepared under these conditions, we successfully replicated features as small as 100 nanometers. Finally, we varied thiol-ene (specifically the -ene component) composition in order to study etch resistance and toughness.
SECTION D: ORGANIC ELECTRONICS AND NANOPHOTONICS

(16) SELF-ASSEMBLED MONOLAYERS AS COUPLING AGENTS FOR MOLECULAR ELECTRONICS
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In the constant push to decrease the size of electronic devices, the ultimate goal may be to use single molecules as conductors, insulators, or transistors. In this project, bifunctional molecules were explored as possible conducting agents to connect metal electrodes. A series of bridged aromatic disocyanide molecules were synthesized, and self-assembled monolayers were formed on gold and palladium surfaces. These planar, entirely conjugated structures are expected to allow for good conduction of electrons. Ellipsometry measurements of monolayer thickness showed that complete monolayers formed and that molecules were positioned perpendicular to the metal surface. IR spectroscopy showed that that one isocyanide group coordinated with the metal surface and one remained free, as expected.

(17) DIRECT FABRICATION OF ORGANIC ELECTRONICS
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The functional components, thiopheneacetyl-2-oxyethyl methacrylate, 2-methacroyloxyethyl-2’-bromoisobutyrate, or bromostyrene, were dissolved in a stock photopolymer resin, and nano-contact molding was utilized to pattern these resins with features as small as 100 nm. After curing the added functional components provided reactive sites for the growth of poly(3-hexyl-2,5-thiophene) by oxidative polymerization or GRIM polymerization. After brush growth utilizing oxidative methods, the film thickness and feature size were observed to increase by 3.1 nm and 7.0 nm, respectively, and the molded features changed from nonfluorescent to fluorescent. GRIM polymerization led to increases in film thickness of 6.8 nm and feature size of 3.2 nm, and also produced fluorescent features after brush growth. The materials presented are characterized by GPC, AFM, ellipsometry, UV-vis spectroscopy, water contact angle, and fluorescence microscopy.

(18) RELATIONSHIP BETWEEN MOLECULAR WEIGHT, MORPHOLOGY AND CHARGE TRANSPORT IN REGIOREGULAR POLYTHIOPHENE
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Regioregular poly (3-hexylthiophene) (P3HT) is one of the leading candidates replace amorphous silicon as the active layer of low-cost thin-film transistors. We have studied the effect of molecular weight on charge carrier mobility and film morphology in thin film polymer transistors and space charge limited diodes made from P3HT. We have observed a substantial increase in mobility with increasing molecular weight in both structures. We have also observed relationships between mobility and annealing, casting solvent, and casting method. We have used atomic force microscopy and grazing incidence x-ray scattering to identify the dominant changes in morphology and relate them to these changes in charge transport.

Section D
(19) CHARACTERIZATION OF SELF-ASSEMBLED GOLD NANOPARTICLE MONOLAYERS
FOR SOLID SATE MEMORY DEVICES
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The phenomenon of bistability in organic switches provides an alternative form of non-volatile solid state
memory. We propose a device in which an organized monolayer of 5 nm Au nanoparticles is assembled
between two semiconducting layers. The presence of the Au monolayer creates bistability in which two
different resistance states are achieved at a given voltage. Au colloid stabilized with 1-dodecanethiol in
toluene was characterized with XPS and TGA to confirm concentrations. FTIR and NMR analyses were
supplemental in determining the amount of 1-dodecanethiol attached to Au and in excess. TEM imaging
yielded evidence of initial hexagonal close pack ordering of Au monolayer. Techniques for increasing
surface coverage by nanoparticles are currently being investigated to develop a reproducible technique for
future device fabrication.

(20) 3-D FDTD FOR NANOPHOTONICS DEVICE OPTIMIZATION
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The finite difference time domain (FDTD) approach is now widely used to simulate the expected
performance of photonic crystal, plasmonic, and other nanophotonic devices. Unfortunately, given the
computational demands of full 3D simulations, researchers can seldom bring this modeling tool to bear on
more than a few isolated design points. Thus, 3-D FDTD as it stands now is merely a verification rather
than a design optimization tool. We use several coarse grid algorithms that retain the flexibility of FDTD,
have high accuracy for modeling small spatial features and reduce computation times. We compare these
four different strategies with normal staircasing errors and report results that will be useful information to
the active FDTD/nanophotonics community. Also, improvements in the way the dispersion relation is
obtained allow us to fine tune the results and account for errors arising in band diagrams due to
degeneracies in a general, non-specific way.
SECTION E: BLOCK COPOLYMERS AND GELS

(21) FUNCTIONAL POLYMERS AS BUILDING BLOCKS TO NANOSTRUCTURES
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Functionalized polymers can serve as building blocks to a wide variety of technologically important nanostructures such as nanocomposites and nanoparticles. We have investigated the controlled synthesis of magnetic nanocomposites comprising a cobalt nanoparticle (ca. 10 nm in diameter) surrounded by an amine functionalized polymer coating. These cobalt based nanostructures show great promise in magnetic storage and diagnostic applications. In a similar fashion, block copolymers of a novel imidazolium polyelectrolyte and polyethylene oxide form nanometer sized micelles (ca. 20 nm in diameter) in water and the specifically tailored ionic liquid core can be used for catalysis reactions. Finally we have prepared block copolymers containing an acidic functional groups and hydrophobic styrene units. These structures form shell-cross linked nanoparticles (ca. 30-100 nm in diameter) which are viable drug delivery agents and diagnostic structures for cancer therapy.

(22) COMPLEX ARCHITECTURES IN BLOCK COPOLYMERS
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The architecture of block copolymers plays an important role in not only their microstructure but also their bulk properties. Consequently, complex architectures hold promise of not only novel physics but also novel materials. Two such efforts involve crosslinked block copolymers and amphiphilic tetrablock copolymers. Even though copolymers can exhibit temperature-induced microstructural transitions (order-disorder transitions), it can be difficult to exploit this phenomenon due to the liquid-like nature of the disordered state. We have discovered that by crosslinking one component of a block copolymer we can preserve the order-disorder transition at a specific, narrow range of crosslinking density. Furthermore, we find that the symmetry of the ordered phase plays an important role in the grain structure as confirmed by depolarized light scattering and transmission electron microscopy. There is much interest in understanding the role of molecular structure in the aggregation behavior of amphiphilic molecules in water. Although all biological membranes are composed of a bilayer, we have created a double-amphiphile synthetic macromolecule to create locally-planar monolayer aggregates in pure water. We characterize the properties of our polymer in solution using dynamic light scattering and light microscopy.
(23) EFFECT OF ARCHITECTURE ON THE SELF-ASSEMBLY OF BLOCK COPOLYMERS AT INTERFACES: LINEAR-NANOPARTICLE VS. LINEAR AB DIBLOCKS

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We have synthesized a series of poly(ethylene glycol)-b-(styrene-r-benzocyclobutene) (PEG-β-(S-r-BCB)) block copolymers with different architectures. The linear block copolymer precursor and the linear-nanoparticle block copolymer resulting from selective intramolecular crosslinking of the BCB units have exactly the same molecular weight and chemical composition, but different architectures which depend on the degree of crosslinking in the S-r-BCB block. The thermal and structural changes in the bulk state of the block copolymer after the intramolecular crosslinking reflect the rigid, globular shape of the nanoparticle block whose properties vary as a function of crosslinking density. The block copolymers are shown to self-assemble into dramatically different surface aggregates at the air-water interface: while the linear block copolymer forms disk-like surface assemblies over the range of compression states, the nanoparticle-linear block copolymer exhibits long (> 10 μm) worm-like aggregates whose length increases as a function of increasing crosslinking density. The driving force behind the morphological change is thought to be the restricted degree of stretching of the nanoparticle block due to the intramolecular crosslinking.

(24) MECHANICAL PROPERTIES OF POLY(ETHYLENE GLYCOL) DIACRYLATE/POLY(ACRYLIC ACID) (PEG-DA/PAA) DOUBLE NETWORKS (DN) SYNTHESIZED FOR USE AS ARTIFICIAL CORNEAS

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Polymerizing poly(acrylic acid) (PAA) within poly(ethylene glycol) diacrylate (PEG-DA) single network (SN) hydrogels yielded optically clear 50% PEG-DA/50% PAA double network (DN) hydrogels. The DN hydrogels were synthesized by a two-step method using photopolymerization with ultraviolet (UV) light. The resulting DN hydrogels and component networks were characterized by uniaxial tensile testing and water content studies. The tensile strengths and Young’s moduli of the DN hydrogels composed of 50% PEG-DA and 50% PAA were larger than those of either SN. Furthermore, the water contents of the 50% PEG-DA/50% PAA DN hydrogels were comparable to those values of a human cornea. By maintaining nutrient permeability as well as high mechanical strength and water content, the optically clear 50% PEG-DA/50% PAA DN hydrogels represent a promising class of biomaterials for use as artificial corneas.
SECTION F: MOLECULAR DYNAMICS SIMULATIONS

(25) TAIL CORRECTIONS TO VAN DER WAALS POTENTIALS: IMPROVED ACCURACY AND EFFICIENCY IN MOLECULAR DYNAMICS SIMULATIONS
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Using “classic” Lennard-Jones potentials for Argon atoms, we investigate the effects of the well-published but somewhat unknown and underused tail corrections to potential energy and pressure. In standard MD simulations, potentials are truncated or smoothed to zero beyond a certain distance for computational efficiency. This procedure introduces a noticeable shift in the total potential energy and pressure of the system. In a constant pressure ensemble, these shifts produce changes in the thermal, dynamical, and structural properties of the system, as we verify by comparing the results of simple simulations computed with and without the tail corrections. Overall, we find significant differences between the thermal properties of the corrected versus uncorrected potentials. In addition, we find that measured properties preserve accuracy in corrected potentials as the number of simulated atoms decreases, a result that implies that molecular dynamics simulations may employ tail corrections to enhance the accuracy and computational efficiency of molecular dynamics simulations.

(26) MOLECULAR DYNAMICS SIMULATIONS OF WATER UNDER SUPERCRITICAL CONDITIONS
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In order to accurately simulate protein folding, the protein must be placed in an environment similar to one in which it would be found in the body, which comprises of approximately 85% water. Much research has gone into improving this water model in order to cut down on processing time and to generate more accurate results. The water model commonly used by the researchers here at IBM was investigated under supercritical conditions and compared to a widely accepted equation of state for water. Also, comparisons were made between separate simulation runs conducted at different pressures and temperatures.
(27) SELF-ASSEMBLING NANOSTRUCTURED MATERIALS: SIMULATING THE KINETICS OF FOLDAMERS
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We apply several methods to probe the ensemble kinetic and structural properties of a model system of poly-phenylacetylene (pPA) oligomer folding trajectories. The kinetic methods employed included a brute-force accounting of conformations, a Markovian state matrix method, and a non-linear least squares fit to a minimalist kinetic model used to extract the folding time. Each method gave similar measures for the folding time of the 12-mer chain, calculated to be on the order of 7 ns for the complete folding of the chain from an extended conformation. Utilizing both a linear and a non-linear scaling relationship between the viscosity and the folding time to correct for a low simulation viscosity, we obtain an upper and a lower bound for the approximate folding time within the range 70 ns < t < 350 ns. This is in agreement with the experimentally measured folding time on the order of 160 ns. The kinetic model used to fit the kinetic behavior of the ensemble of trajectories provides a framework to describe the bulk folding mechanism. We were able to identify two unique clusters of conformations that provide a structural basis to account for the appearance of a kinetic intermediate in the mechanism. We discuss the implications of these findings in the context of Helix-Coil Theory.

(28) TRANSLATING PROTEIN FOLDING RESEARCH FOR STUDENTS AND THE GENERAL PUBLIC
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The objective of this project is to translate current research into teacher and community friendly concepts. Large interactive models and an informative kiosk are being constructed for exhibit at the San Francisco Exploratorium. Lessons plans have been developed that exhibit this research of Dr. Pande, in the area of distributive computing to model protein folding. The exhibit and the lesson plans will give others access to the fundamentals and the actual research of Dr. Pande.
(29) LOW ENERGY ARGON ION MILLING OF FOCUSED ION BEAM SAMPLES PREPARED FOR TRANSMISSION ELECTRON MICROSCOPY ANALYSIS
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Focused ion beams (FIB) are increasingly utilized to prepare a wide variety of samples for SEM and TEM analysis. FIB use a 30 keV Ga liquid metal ion source to mill a sample. FIB are known to cause amorphization to the top 30nm of a sample although this can be minimized by decreasing beam current. In addition, changes in the surface chemistry of a sample occur due to the Ga+ ion beam. Amorphization and changes in surface chemistry can be problematic for TEM analysis of multilayer crystalline structures. Decreased signal to noise due to amorphization of a sample decreases the ability to resolve crystal structure and determine lattice spacing. Recent developments in a separate low energy Ar ion beam polishing step have proved useful for traditional sample preparation. Low energy Ar ion beams of 200 to 2000 eV are used to prepare thinner TEM samples and remove damage from higher energy precision ion polishing systems. The goal of this work is to evaluate the use of a low energy Ar+ beam to remove damage and prepare thinner, more ideal, FIB prepared samples for TEM analysis.

(30) EXPLORING CHANGES IN DEBOND ENERGY OF HUMAN STRATUM CORNEUM RELATIVE TO PH
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The outermost layer of the skin, the stratum corneum (SC) provides the first mechanical and diffusion barrier to the environment. The SC has a pH gradient ranging 5 to 7 from the outside to the inside. In situ, the SC is often exposed to substances outside of this natural range, such as soaps (pH 10) that cause SC swelling and can result in skin irritation. Understanding how the SC cohesive properties change with pH will aid in the design of skin products. Specimens were soaked in three different pH buffered solutions (pH 4.7, 6.7, 9.9) with constant ionic strength (0.006 M). Double-cantilevered beam fracture tests were performed to determine the debond energy (G) of the treated SC. G is a measure of the energy required to propagate a debond through the SC. The G-value of the control case was 4.4±1.1 J•m\(^{-2}\) (average±standard deviation). The G-values all increased after treating to 4.5±1.7, 5.2±1.2, and 4.6±1.7 J•m\(^{-2}\) for the acidic, neutral, and basic pH treatments, respectively. Despite increases in the lipid melting temperature with increased pH, the G-values were statistically indistinguishable. The constancy of debond energies with lipid changes suggests that other components of the SC contribute more significantly to the cohesive properties.
(31) A SAMPLING OF NEW HARDWARE IN INDUSTRIAL AUTOMATION CONTROL
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This summer’s work has centered on the use of newly acquired hardware to simplify the use and maintenance of equipment at the IBM Almaden facility. Opto22\textsuperscript{TM} hardware has been programmed with flowchart logic to operate remote seismic sensors that will protect facilities management machinery in the case of an earthquake. Flat touch-screen monitors have been tested and equipped to run simple debugging code written expressly for “spintronics” equipment at the IBM Almaden Research Center. These two systems have been investigated and learned totally this summer in an attempt to increase the efficiency with which equipment is operated and maintenance and can be performed.

(32) TEOSINTE CROSSING BARRIER
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Wild teosinte and cultivated maize are members of the same species. They are able to cross pollinate in laboratory conditions. A teosinte gene or gene cluster has been found to inhibit crossability with domesticated maize in the wild. This gene or gene cluster causes nonreceptivity to pollen of other maize varities. By using known markers in chromosome 4, 5, and 6, we will be able to systematically narrow down the location of the Tcb1 gene. Results for the locus of the Tcb1 gene are still on going. Through fine mapping the location of the Tcb1 gene will be narrowed down to a specific location. With a better understanding of how this crossing barrier works, researchers may be able to develop techniques to prevent unwanted hybridization in agricultural fields.
SECTION H: POLYMER DYNAMICS

(33) USING BIREFRINGENCE TO ANALYZE DNA SOLUTIONS IN EXTENSIONAL FLOW
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The birefringence of DNA solutions of varying concentrations under different extensional flow strengths was measured in this experiment. This was done in an attempt to characterize the forces and interactions on the individual DNA chains, and individual polymers in general, under different flow intensities. Unlike in more concentrated regimes, the polymers in the dilute solutions do not experience significant intermolecular interactions and mainly the effects of the flow are considered. The birefringence was measured using a polarization modulated flow birefringence instrument. The birefringence of a solution is dependent upon the orientation of the individual DNA chains. As the chains become more aligned, anisotropy increases, which, in turn, increases the birefringence of the solution. This work will be used in conjunction with single polymer studies in order to get a more complete picture of the effect of flow on polymer motion.

(34) SINGLE POLYMER DYNAMICS IN CONCENTRATED SOLUTIONS OF DNA
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The behavior of polymers highly depends on solution concentration. Polymer motion in the concentrated regime is qualitatively different from that in dilute cases due to the entanglements that occur between polymer molecules. The traditional theoretical starting point for studying polymer behavior in concentrated solutions is “reptation theory” put forth by Doi, Edwards and deGennes. Subsequent modifications to this theory, guided by complementary experimental work, have resulted in an increasingly better representation of real systems (ex. the experimentally observed scaling law, $\tau \sim M^{3.4}$, can now be theoretically explained by incorporating the phenomena of “constraint release” and “contour length fluctuation” into reptation theory). It must be noted that most experimental data is of the bulk nature, where individual molecular behavior is hidden behind ensemble averaged quantities. Recently, single polymer experiments have been used to successfully visualize and extract molecular DNA data in dilute solutions. This study aims at using the experimental framework of these single polymer studies to observe single DNA molecules and analyze their behavior in systems of high concentration. Data acquired during step-strain experiments will allow us to examine the relaxation of entangled DNA and planar extensional flow experiments will help us understand the interaction of flow and polymeric motion in concentrated solutions.
(35) VISUALIZATION OF SINGLE POLYMER DYNAMICS USING FLUORESCENT POLYSTYRENE

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In this work, we extend the realm of single molecule visualization of polymers to synthetic systems. Fluorescence microscopy is used to visualize single polystyrene molecules in a Boger fluid. To date, single molecule experiments have only been carried out on biological polymers such as DNA, which is more rigid (larger kuhn step size) than synthetic polymers. For synthetic polymers such as polystyrene, the ratio of kuhn step size to molecular diameter is on the order of unity, which leads to an increased importance of intramolecular interactions (hydrodynamic and excluded volume). In the past, experiments performed on synthetic polymers have been restricted to macroscopic flow measurement techniques. We are constructing new flow cells to study the behavior of single polystyrene chains in planar extensional flow. Data collected from these images will be used to study the characteristics of highly flexible polymer chains. With the ability to study single chains, phenomena such as a conformational hysteresis can be analyzed. Computer simulations using Brownian dynamics techniques will then be performed to verify the presence of such phenomena.

(36) A RHEOLOGICAL STUDY OF TWO-DIMENSIONAL POLYMER MELTS

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When molecules of the flexible polymer poly(tert-butyl methacrylate) (PtBMA) are confined to the air-water interface, the resulting arrangement can be thought of as a two-dimensional polymer system. The rheological properties of monolayers of PtBMA with molecular weights ranging from 80,000-780,000 g/mol will be presented. Surface shear moduli were measured over a range of frequencies using an interfacial stress rheometer such that important time scales in the system could be identified. Creep compliance experiments were also conducted to explore the dependence of retardation time and surface shear viscosity on molecular weight. Furthermore, changes in the rheological properties of these monolayers as surface pressure was varied were correlated to phase transitions observed during compression isotherms. A theory addressing the relationship between observed mechanical properties and the molecular structures of the polymeric films will also be offered.
SECTION I: BIOMOLECULES AT INTERFACES

(37) HYBRIDIZATION WITH NANOSTRUCTURES OF SINGLE-STRANDED DNA: A FUNDAMENTAL STEP TOWARDS SENSITIVE DNA DETECTION AND CONSTRUCTION OF COMPLEX DNA ARCHITECTURES ON SURFACES

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Nanostructures of single-stranded DNA (ssDNA) were produced within alkanethiol self-assembled monolayers using nanografting, an atomic force microscopy based lithography technique. Further, varying the fabrication parameters such as the concentration of ssDNA and grafting force can control the density of ssDNA molecules within nanostructures. The DNA molecules within nanostructures remain active and are able to bind with the complementary strands. The label-free hybridization of nanostructures, monitored using high-resolution AFM imaging, is proven to be ultrasensitive as few as 54 molecules can be detected. Ex situ and in situ label-free hybridization and control experiments reveal that the DNA nanostructures have high selectivity towards the complimentary DNA. The efficiency of the hybridization reaction at the nanometer scale highly depends on the ssDNA packing density within nanostructures. The hybridization is optimal at packing density range from $0.16 \times 10^{13}$ to $0.4 \times 10^{13}$ molecules/cm$^2$, but decreases dramatically at the packing density of $1.2 \times 10^{13}$/cm$^2$ or higher. This study represents the first step towards construction of complex DNA architectures on surfaces, and regulating the hybridization reaction of DNA nanostructures.

(38) CHARACTERIZATION OF BIOMOLECULES ON ULTRATHIN POLYMER FILMS

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Knowledge of surface effects on adsorbed molecules is critical for the further tailoring of nanostructures for biotechnological applications. The interaction of several biomolecules with polymer surfaces was studied by measuring and comparing the adsorbed macromolecules’ conformations on polymers and on mica. Monolayers of 2-[methoxy-(polyethyleneoxy)propyl]trimethoxy silane, covalently grafted onto silicon wafers, were characterized using ellipsometry, atomic force microscopy (AFM), and contact angle measurements. Thin layers of polydimethylacrylamate containing 4% benzocyclobutane spun cast on silicon wafers and cross-linked were characterized using the same techniques, and their properties of film thickness, roughness and wettability were compared. The modification of AFM probes with the two polymers was also studied by means of AFM force-distance curves. Adsorption of Streptavidin, biotinylated DNA and Streptavidin- biotinylated DNA complexes on these thin polymer films and on mica was investigated by AFM and fluorescence microscopy to reveal the different spreading and aggregating effects of the surfaces on the biomolecules. The average height of the biomolecules absorbed on polymer films was significantly less than on mica and their width was greater, suggesting that the polymers exhibit a stronger attraction and spreading effect compared to mica.
Current and future work to investigate the behavior of enzymes with surface-bound substrates are described. These reactions are important in applications such as detergents and food processing. The reaction of a serine protease with a tethered protein substrate indicates that surface diffusion may play an important role. Direct imaging of surface diffusion is desired. Fluorescence microscopy is a simple, rapid and high resolution method that uses labeled materials. Both ellipsometric and surface plasmon resonance (SPR) imaging provide sensitive surface measurements in real time, with unlabeled reagents. Utilizing microfluidic setups with all these techniques, we have obtained fluorescent images and preliminary pictures from ellipsometric and SPR imaging.

Lung surfactant (LS) facilitates normal respiration in humans by countering forces that would otherwise cause alveolar collapse on exhalation. A lack or disruption of LS can therefore cause breathing to be more onerous as exhibited in Respiratory Distress Syndrome (RDS) in infants and Acute Respiratory Distress Syndrome (ARDS) in adults, respectively. LS is a complex mixture of proteins and phospholipids generated by Type II alveolar epithelial cells. Recent studies indicate that airborne pollution particles can damage these cells, leading to apoptotic events. It is not known how the cellular components released during the cell death cycle affect the function of LS. To investigate, we spread monolayers of a commercially available lung surfactant replacement, Infasurf, on novel subphases to simulate physiologic conditions. We have substituted the widely used saline subphases with cell culture supernatants of human lung epithelial A549 cells exposed to varying conditions, including residual oil fly ash (ROFA) particles emission-source airborne pollution particles that cause cellular damage. Fluorescence microscopy and a Langmuir-Wilhelmy balance were used to characterize these systems. Novel structures and interactions were observed.
SECTION J: SURFACES AND ULTRATHIN FILMS

(41) CHARACTERIZATION OF POLYCONJUGATED THIN FILMS SYNTHESIZED BY HOT WIRE CHEMICAL VAPOR DEPOSITION
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We are exploring the use of hot-wire chemical vapor deposition (HW-CVD) as an alternative, solvent-free technique to produce compact polyconjugated films from vaporized monomers. Monomers investigated include aniline, benzonitrile and thiophene, and it is found that polymeric films can be grown by different sets of reactor conditions. In one set of conditions, the hot wire is a low-melting point metal that serves as a continuous source of evaporated catalyst. Films grown using this scheme incorporate significant amounts of evaporated metal. The second scheme is more typical of HW-CVD processes, utilizing a hot refractory metal and gas-phase collisions to activate precursors. The use of gas-phase radical initiators has also been explored. Infrared, X-ray photoelectron and UV-visible absorption spectra have been obtained to characterize the structure of HW-CVD films produced by these methods. The different CVD schemes are found to rely on different chemical mechanisms for polymerization and growth.

(42) AUTOMATION OF VAPOR DEPOSITION POLYMERIZATION (VDP) SYSTEM FOR GRAFTING OF POLYPEPTIDES ON PLANAR SOLID SUBSTRATES
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Vapor deposition polymerization (VDP) of N-carboxy anhydride (NCA) has been proven to be an effective method of synthesizing various surface-grafted homopolypeptides and block copolypeptides with controllable thickness and composition. (Y. Chang 1998; Y.L. Wang 2002; W. Zheng, 2003) For surface-grafted poly-benzyl-L-glutamate (PBLG) on the silicon surface, the degree of polymerization up to 2000 can be achieved using VDP as compared to only 300 for melt and solution polymerization. Compared to the best results on the Si-PBLG system reported by Wang and Chang at UC, Irvine in 2002, we can now synthesize almost the same thickness chemisorbed PBLG film (181nm) at triple growth rate with higher homogeneity(thickness STD=3nm) and greater chemisorbed content (73%). We also developed a real-time tracking method known as VDP reaction profile (VDPRP) to make us more able to study the VDP mechanism and control the VDP process. However, several technical limitations of the current VDP system prevent us from controlling and monitoring the pressure in the VDP reaction region and temperatures of the substrate and monomers accurately over a wide range. Therefore, we are now developing a new VDP system, including LabVIEW control, redesigned high vacuum system and thermal VDP setup inside the vacuum chamber. The redesigned heating plates will extend the temperature control range from less than 120°C up to 316°C with much higher accuracy (less than 1 °C). The redesigned vacuum system will allow us to measure the pressure much closer to the VDP region. Finally, a customized software application programmed through LabVIEW will integrate all three parts.
(43) DEWETTING KINETICS IN ULTRATHIN POLYMER FILMS: THE EFFECT OF POROSITY AND NANOPARTICLES
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Studies show that films above their glass transition temperatures (T_g) undergo significant disruption known as dewetting. The studies presented show how nanoparticle additives on this thin film affect the dewetting behavior. We studied the effects using a bilayer system comprised of polystyrene (PS) on top of poly(methyl-methacrylate) PMMA film. The nanoparticles are silica particles that show drastic distinction in the surface roughness of the film surface. The porosity studied in the film is the effect of the removal of the silica particles. Aiming to optimize the dewetting suppression PS films dewetting kinetics were obtained by optical microscopy imaging, revealing the critical percent rate concentration of nanoparticles required for the suppression of dewetting PS films. Further analysis was done through atomic force microscopy (AFM) to obtain insight on the suppression behaviors due to nanoparticles during dewetting.

(44) ORIENTATIONAL ORDER & DYNAMICS OF POLYMERS IN ULTRA-THIN FILMS
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The orientational order and self-diffusion of polymer chains have been measured in ultra-thin (5–50 Å) films of a perfluoropolyether (PFPE) by 19F NMR. PFPE films are used as industrial lubricants in the thickness range of 10–20 Å. Two-dimensional experiments have been used to correlate the residual dipole–dipole couplings with isotropic chemical shifts for the –(O–CF2–)– units. Fitting these spectra yields a Saupe order parameter, Szz, which is a measure of polymer segment orientation with respect to the film normal. The order parameters for the thinnest films (~5 Å) are approximately 0.12, which indicates a high degree of orientational order for the polymer backbone. The diffusion coefficients of PFPE films have been measured by pulsed field gradient (PFG) NMR techniques. Due to the thinness of the films, diffusion can be neglected in the direction of the surface normal, and the measured diffusion coefficients correspond to center-of-mass diffusion in the plane of the film. The diffusion coefficients obtained for different thicknesses are compared to the isotropic self-diffusion coefficient measured on the bulk liquid polymer. The measured order parameters and diffusion coefficients demonstrate that ultra-thin PFPE films form a highly orientationally ordered liquid phase.

(45) INVESTIGATION OF SURFACE TENSION OF RUBBER AFTER MECHANICAL STRETCHING
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This poster describes the systematic investigation of surface tension by utilizing contact angle measurements on different polymers as a function of polymer stretching. Interfacial tension may be extracted from advanced contact angle measurements using Young’s equation. This measurement is significant in the application of elastomer materials. Results may be used as a guide in using elastomeric polymers for microfabrication, surface modification, and advanced material synthesis.
SECTION K: INTERFACIAL TECHNIQUE DEVELOPMENT

(46) POLARIZATION-MODULATED SECOND HARMONIC GENERATION IMAGING AND CHARACTERIZATION OF ANISOTROPY OF BIOLOGICAL SYSTEMS

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Polarization-modulated second harmonic imaging (PM-SHG-I) is a well demonstrated method for quantifying disorder of collagen tissue structures. It is nondestructive and allows people to perform in vivo study of collagen tissues up to a depth of 200-300 microns with the highest resolution of ~ 1.5 microns. Second harmonic generation is a two photon absorption process which generates new photons at twice the original frequency. Due to the non-centrosymmetry constraints, SHG is particularly effective in identifying fibrillar structures organized on the scale of wavelength of light within soft tissues. In this study, regions of interest (ROI) within the collagen samples are identified and extracted using texture segmentation techniques. The anisotropy of different structures is quantified with Gabor wavelet which extracts the orientation information at different spatial frequencies and the result is consistent with the direct secant method.

(47) DESIGN ON AN INTERFACIAL DIELECTRIC PROBE

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A microwave probe consisting of a coplanar transmission line on a glass substrate was developed in order to measure the binding of biomolecules at a liquid-solid interface. The probe operates by measuring changes in the dielectric properties of the transmission line due to the interface binding of the biomolecules. The sensitivity of the probe to operating temperature, frequency, saline volume and saline molarity was studied using numerical models that simulate a transient pulse propagating through the probe. The results of the numerical models indicate that the propagation and attenuation in the probe are sensitive to changes in each of these parameters. Finally, a finite difference model was used to explore the spatial distribution of the electromagnetic fields within the probe. The effective sampling area of the probe was shown to be confined within areas concentrated at the edges of the electrodes that extend approximately 10 microns into the saline region between the electrodes.
(48) MICROWAVE TRANSMISSION LINE DIELECTRIC PROBE TO DETECT MACROMOLECULAR SURFACE INTERACTIONS
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A probe is being developed to detect biomolecular binding events at a liquid-solid interface in the microwave regime in real-time and without using fluorescence labels. The essential part of the probe is a coplanar transmission line (CTL) fabricated on a glass slide that can detect the dielectric changes in close proximity of an interface. The CTL geometry concentrates the electric flux density in the gap region between the signal and ground electrodes and makes it very sensitive to permittivity changes at the liquid-solid interface. The probe operation was demonstrated by detecting the protein A and rabbit IgG binding at concentration levels on the order of 10pg/mm². We have also shown that the probe can follow the in-situ polyelectrolyte deposition of multiple layers onto a glass surface. Atomic force microscopy and fluorescence were used to confirm the surface reactions.

(49) DEVELOPMENT OF FORCE PROBES FOR STUDYING TOUCH SENSATION
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We as human beings depend greatly on the sensory nerve cells that govern our sense of touch. If such cells cease to function properly, we may lose the ability to respond to another’s touch or be unable to respond to a more painful and potentially damaging event—such as stepping on a tack. Reduced touch sensation, or peripheral sensory neuropathy, is especially common in people with diabetes and can be caused by chemotherapy treatments as well as several other diseases, including AIDS. Force probes that can detect the first signs of impaired touch sensitivity have the potential to improve diagnosis of DPN and target patients for more aggressive diabetes treatment before the onset of neuropathy. Such force probes may not only improve the life of diabetics, but also produce a significant cost savings. Current methods are based upon von Frey’s method of fiber buckling to assay responses to defined forces and deliver forces of ~100 µN. Improved, portable force probes that can deliver smaller forces (1-10 µN) have the potential to improve diagnosis of peripheral sensory neuropathy.
SECTION L: LIPID BILAYERS

(50) PREPARATION-DEPENDENT VESICLE AGING EFFECTS ON VESICLE FUSION AND BILAYER FORMATION

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We would like to understand and control the process of vesicle fusion on solid substrates. To model this process, we are studying single lipid component vesicles containing 1-Palmitoyl-2-Oleoyl-sn-Glycero-3-Phosphocholine (POPC), which is typical of many biomimetic systems used in this field. We are using dynamic light scattering to characterize the evolution of vesicle size during the time period following the preparation of the vesicles by extrusion through a polycarbonate membrane. We have examined vesicles between 30 and 100 nm in diameter and have discovered a contraction in size as a function of time. Such a contraction may reflect a densification of the lipid bilayer forming the vesicle shell, which could result from the shearing force stored in vesicles during the extruding process. Meanwhile, vesicles formed by sonication have not shown this time-dependent behavior. This trend could prove useful for controlling the subsequent interactions with the solid substrate.

While the dynamic light scattering measurements have provided information on vesicle size, we also desire a method for describing the kinetics of vesicle adsorption and fusion on solid substrates. Using a quartz crystal microbalance with dissipation, we have been able to monitor adsorption kinetic behavior as a function of aging. These results discern adsorbed, but intact, vesicles from ones that had fused with the substrate to form a planar bilayer, depending on the vesicle age. Specifically, aged vesicles clearly show reduced adsorption kinetic times as well as lowered dissipation values. In general, the frequency and dissipation values approach those obtained from equivalent diameter, sonicated vesicles. The question then arises of whether it is possible to control vesicle adsorption kinetics. Such kinetic behavior suggests that vesicles are dynamic systems that must be controlled depending on the experimental purpose. Additionally, vesicle fusion kinetic behavior could be controlled to study short-lived intermediate structures in the vesicle fusion process.

Tapping mode atomic force microscopy (TM-AFM) measurements have also been performed to clarify the relationship between the adsorption of vesicles on the solid surface and the bilayer formation. Bilayers formed from extruded vesicles show a clear transition in homogeneity after aging nine days. This correlates with mass uptakes and kinetic changes seen in the QCM results. The driving forces for these changes are currently being pursued.
(51) INFLUENCE OF VESICLE SIZE ON THE FORMATION OF SUPPORTED LIPID BILAYERS
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We used lipid bilayers supported by silicon oxide to model the structure of biological membranes. To install bilayers, we used unilamellar vesicles produced by extrusion of multilamellar POPC vesicles through polycarbonate filters. After characterization by Dynamic Light Scattering (DLS), the vesicle solutions were flowed over a piezoelectric quartz crystal coated with SiO₂. An oscillating electric field was applied, allowing us to follow the vesicle adsorption and rupture process via deviations in the crystal’s resonant frequency. To measure the viscoelastic properties of the supported bilayer and intermediate structures, we monitored the rates at which resonance decayed upon interruption of the driving voltage. Finally, using a technique called Fluorescence Recovery After Photobleaching (FRAP), we compared the fluidities of fluorescently labeled bilayers formed from vesicles of different sizes (diameters 63 – 529 nm). We report mobilities of 1.00 – 1.31 μm²/s for bilayers formed from large parent vesicles (150 – 529 nm) and 1.62 – 1.76 μm²/s for those formed from vesicles with smaller diameters (63 – 150 nm).

(52) PH DEPENDENCE OF LIPID VESICLE DEPOSITION: ADSORPTION KINETICS AND DIFFUSIVITY ON A SILICA SURFACE
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The fusion and spreading of phospholipid bilayer membranes on silica surfaces was investigated as a function of pH. As analytical tools the Quartz Crystal Microbalance-Dissipation (QCM-D) and Fluorescence Recovery After Photobleaching (FRAP) were utilized. Our results show that three different adsorption regimes exists; for low pH (4-6) a one-step process for bilayer formation, for intermediate pH (7-9) a two-step process adhesion of vesicles followed by bilayer formation and last for high pH (9-10) vesicle formation. The results clearly show that dispersive and electrostatic forces dominate the processes of bilayer formation and how easily the bilayer process can be manipulated. In the second part we confirmed the different structures with FRAP and analyzed the different measured diffusivity values over the whole pH range. This we compared to the values from the dissipative measurements from the QCM-D. These results are the beginning of an extensive study on the creation of lipid bilayers on planar supports and the different factors that influence this process.
(53) STUDY OF VESICLE FUSION PROCESS BY SIMULTANEOUS MEASUREMENTS OF SURFACE PLASMON RESONANCE (SPR) SPECTROSCOPY AND QUARTZ CRYSTAL MICROBALANCING WITH DISSIPATION (QCM-D)
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The kinetics of vesicle fusion on a planar surface followed by the formation of a bilayer membrane is not yet fully understood. There are different possible scenarios for lipid vesicle surface interactions; therefore identifying and characterizing these situations is important. Lipid bilayer formation has previously been investigated through various techniques including surface plasmon resonance spectroscopy (SPR) and quartz crystal microbalancing with dissipation (QCM-D). These two techniques are now combined in one experimental setup to produce simultaneous measurements on the same sample. This provides a more complete picture of vesicle fusion than either technique alone. Using commercial QCM-D gold sensors, a grating coupler was etched onto the surface. A self-assembled monolayer (SAM) of 2,3-di-O-phytanyl-sn-glycerol-1-tetraethylene glycol-D,L-α-lipoic acid ester (DPTL) was then formed. The production of a tethered lipid bilayer (tBLM) from the fusion of diphytanoylphosphatidylcholine (DPhyPC) liposomes to the SAM was observed. In this novel approach of simultaneously using SPR and QCM-D, further molecular structural information of this process is provided.

(54) A DIRECT COMPARISON BETWEEN THREE DIFFERENT QUARTZ CRYSTAL MICROBALANCES UNIQUE TO THE CPIMA LABORATORY
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The objective of this study was to draw a direct comparison between three different quartz crystal microbalances (QCM) in order to correlate resistance and dissipation to theory. Three different QCMs, Resistance, Impedance and Dissipation were used for this experiment. Each QCM measured mixtures of water and glycerol ranging from 0-100%. Decreases in resonant frequency proportional to the density and viscosity of the solutions measured were observed. As a result, we were able to compare the observed frequency shifts, resistance, and dissipation to theoretical values for the solutions measured. Deviations from theoretical values were determined and used to compare both the advantages and disadvantages of each instrument.
Combining atomic force microscopy (AFM) and fluorescence recovery after photobleaching (FRAP), we have found that the inter-monolayer coupling of phase-separated supported bilayers formed by vesicle fusion can be controlled by the method of vesicle preparation. We also find that bilayers with partially asymmetric coupling are metastable and convert, through lipid flip-flop, to a state where all gel phase lipids occupy the top monolayer. The supported bilayers consisted of phase-separated DLPC and DSPC and were formed by quenched vesicle fusion. Coupled and uncoupled DSPC-rich domains were found to be approximately 1.8 nm and 1.0 nm higher than fluid phase respectively. We determined that when the lipids in vesicles are highly mixed (achieved by tip sonification or extrusion), the process of thermal quenching and vesicle fusion froze the gel/liquid coexisting bilayer at a nonequilibrium state, where DLPC was trapped in quickly frozen gel domains and did not have the time to diffuse to DLPC enriched regions. Within an hour, sub-domains of DLPC in one monolayer formed within and around the DSPC enriched regions. This resulted in a metastable state subsequently causing all of the DSPC to flip to one monolayer, i.e. became completely uncoupled. The rate constants of this transmembrane movement were determined and were found to be highly related to the interfacial line tension between different phases. On the contrary, when vesicles with less degree of lipid mixing (achieved by thermal annealing extrusion) were used to form the supported bilayers, only coupled DSPC domains were formed and they did not convert to uncoupled domains for at least several days. These domains appeared to contain no sub-domains of DLPC. We relate these stable and metastable states to hydrophobic mismatch and the state and energy of mixing.

Planar supported phospholipid bilayers (SLB) are well-established experimental systems that are widely used in basic research as well as in the biotechnological industry. In more recent studies SLBs have been utilized to create artificial and hybrid-cell-SLB membrane-membrane junctions. It has been found that the electrostatic environment of the SLB plays a crucial role in the interactions and organization of membrane constituents within these junctions. We novelty use the measurement of electrostatically induced shifts in the emission spectra of potentiometric fluorescent membrane dyes to quantify the net membrane potential at the SLB surface. By varying membrane composition and buffer conditions, we identify the different contributions of the substrate, the membrane constituents and the aqueous solution to the net membrane potential. We find drastic differences (~10nm) in the spectral characteristics of the dye incorporated into free vesicles versus the dye in the SLB, which indicates a strong contribution of the substrate surface charge to the resulting membrane potential. Changing the membrane charge by varying the relative amounts of charged lipid, results in smaller spectral shifts (~1-3nm).
SECTION M: LIPID/PROTEIN INTERACTIONS

(57) HIGH-RESOLUTION IMAGING OF LIPID MEMBRANES WITHOUT FLUORESCENT LABELING
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The lateral organization of the lipid and protein components of cell membranes has recently become an area of great interest, due to the hypothesized existence of “lipid rafts”, which are phase-separated microdomains within the membrane that could play a key role in many cellular processes. Fluorescence microscopy, the conventional method for observing lipid membrane properties, introduces bulky fluorescent labels which may perturb the very organization that they are being used to investigate. Using the NanoSIMS 50, a recently developed system from Cameca Instruments Inc., we demonstrate that secondary ion mass spectroscopy (SIMS), in conjunction with isotopically or chemically labeled membrane components, can be used to elucidate the lateral organization of the membrane through detection of ions unique to each component. Compositional analysis can be performed with sensitivity and lateral resolution that rival fluorescence microscopy, which makes SIMS a potentially powerful tool for the imaging of lipid membranes.

(58) EFFECTS OF GALCER, SPHINGOMYELIN, AND CHOLESTEROL ON DOMAIN MICROSTRUCTURE
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Cellular membranes are not uniform and homogenous as previously thought with the fluid mosaic model. Within the membrane, several different lipids exist, some of which phase separate at physiological temperatures. Recent studies show sphingolipids, glycosphingolipids, and cholesterol phase separate into domains or rafts in cellular membranes. In this study we used a model membrane system to form domains which mimic raft composition. With DLPC as the fluid matrix, we used GalCer, sphingomyelin, and cholesterol in different combinations, to study the unique domains formed. We formed bilayers consisting of six different domain compositions: 1) GalCer, 2) sphingomyelin, 3) GalCer and sphingomyelin, 4) GalCer and cholesterol, 5) sphingomyelin and cholesterol, 6) sphingomyelin, GalCer and cholesterol. Using NBD-PC, a fluid phase lipid probe, we were able to image the domains through florescence microscopy. We found that GalCer forms large domains approximately 20-30 μm, while sphingomyelin forms smaller domains approximately 1-3μm. Bilayers consisting of both GalCer and sphingomyelin exhibit two different domain sizes. One is consistent with the size of sphingomyelin domains (1-3 μm) and the other is consistent with the size of GalCer domains (20 –30 μm), leading us to believe that the two differing domains consist of pure sphingomyelin or GalCer. Any lipid composition that included cholesterol resulted in a bilayer with domain size out of the resolution of optical fluorescence microscopy.
We are interested in studying the multivalent interactions between gp120, an HIV envelope glycoprotein, along with galactose specific lectins Caragana arborescens (CAA) and Trichosanthes kirilowi (TKA) with the receptor lipid Galactosylceramide (GalCer). HIV-1 has two different fusion pathways, which depend largely on cell type. Infection of hepatocytes, sperm cells, vaginal, colonic and neural epithelial cells occur through an initial interaction between gp120 and GalCer, a glycosphingolipid containing a galactose sugar head group. GalCer has been shown to exist on the extracellular leaflet of the cell membrane in nanometer size domains or rafts. The local clustering of GalCer within rafts is thought to facilitate the multivalent interaction between gp120 and GalCer in the initial attachment of HIV-1 to the host cell. It is believed that the display of GalCer ligands within these rafts can affect the strength of the polyvalent interaction between GalCer and receptor protein. We are using supported lipid bilayers to study the effects of GalCer density, mobility and domain size on the binding properties between GalCer and receptor proteins, gp120, CAA and TKA. We have used AFM to image supported bilayers that contain phase-separated domains of pure GalCer and GalCer with the addition of cholesterol. Using slow cooling techniques during bilayer formation GalCer domains can be made to exceed 40 \( \mu \text{m} \) in size, an equilibrium condition. This phenomenon does not occur in bilayers containing cholesterol. GalCer domains containing cholesterol are limited in the 1 \( \mu \text{m} \) to nanometer size range regardless of cooling rates during bilayer formation. This indicates cholesterol alters equilibrium domain size, an effect which is believed to occur in cellular rafts, but has yet to be observed in model membranes. Using fluorescence microscopy we found that gp120 and CAA only bind to nanometer size GalCer domains and GalCer domains containing cholesterol, whereas TKA binds under all domain conditions. This indicates that the micro-structure and display of GalCer within domains can affect the binding properties of the membrane and these effects are protein dependent.
(60) DYNAMIC INTERACTIONS IN IMMUNOLOGY: THE STUDY OF THE DYNAMICS AND RESULTING INTERACTIONS TAKING PLACE BETWEEN T LYMPHOCYTES AND ANTIGEN PRESENTING CELLS
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The movement of T lymphocytes (T cells) and antigen presenting cells (APCs) in the lymph nodes have been studied and modeled using two popular theories. The first theory suggests that the cells move as a result of an attraction between chemicals produced by one cell and the chemoreceptors present on the corresponding cell. A second theory suggests that the movement is solely based on a random-walk-type movement. Our research group has assumed the latter theory in modeling the movement of T cells and APCs using C programs to reproduce results found experimentally. A program was written that allowed for the variation of the number of T cells, APCs, the fraction of antigen-specific T cells, the probability of successful interaction upon contact and the size of the lymph node. In our study, we questioned how changing the parameters of numerous variables affected the time for antigen-specific T cells to find and successfully interact with their specific APC. The effect of moving both the APCs and T cells at varying rates was compared with the case when only T cells were mobile. It was found that the mobility of APCs slightly decreased the time necessary for a successful interaction to occur, but the effect was so small it seems insignificant. Other variables such as cell death and cell activation resulting in the production of Interleukin-2 were studied. We have concluded the project with the production of a 'movie,' an animated sequence of frames, showing the movement and interaction of the T cells and APCs, represented by antigen-specific T cells, antigen-non-specific T cells, specific APCs and non-specific APCs.

(61) CONTROLLING FACTORS THAT INFLUENCE PROTEIN PRODUCTION RATES IN A CELL FREE SYSTEM
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Synthesizing protein via an in-vitro cell free system has several advantages over the standard in vivo methods. Yet to date, producing protein with consistent levels of 1 mg/mL in batch mode has proved elusive. Considerable effort has been spent optimizing the cell free environment to make protein production both efficient and economically viable for eventual larger scale workup. By sustaining protein production rates, high-level protein expression is achieved. We explored the impact of three factors on the rate of protein synthesis in 1mL jacketed bubble column reactors using the Cytomim system. (1) Foaming was observed to noticeably decreases the rate of protein synthesis. By using an antifoam agent to control foaming which occurs by bubbling oxygen into our reaction, protein synthesis was sustained. (2) Bubble affluency requires regulation to stabilize protein synthesis. By calibrating our bubble rate to approximately two bubbles per second, measured improvement was observed in synthesis rates. (3) Replenishment of depleted substrates required for protein biosynthesis is also important. By controlling both the presence of foam, the rate of sparging oxygen, and maintaining critical substrates required for protein expression, the work reported here is an advancement toward sustaining cell free protein synthesis.
SECTION N: TETHERED VESICLES

(62) SEPARATION OF DNA LIPOSOMES USING AFFINITY AND ION EXCHANGE CHROMATOGRAPHY
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Column chromatography techniques can be used for recovery and purification of lipid vesicles based on the number of DNA oligonucleotides incorporated into the vesicle bilayer membrane. This type of vesicle separation is beneficial for differential partitioning of vesicles based on the properties of macromolecules protruding from vesicle membranes. Several different columns and separation methods were used in this study, which took advantage of two properties of DNA – base pair complementation and ionic strength. One method dealt with coupling amino modified DNA oligos to tentagel PEG/PS columns with carboxylic acid functionalities. The coupled single stranded DNA served as a complementary strand to the DNA strands incorporated into the lipid vesicles. Another method involved binding of biotin-functionalized DNA to streptavidin coupled agarose beads. Again, the single stranded DNA coupled to the column served as a complementary strand to the DNA oligos on the vesicles. In both methods non-specific binding of vesicles to the columns caused complications in attaining reliable results. Ion-exchange chromatography was also utilized, however results show that elution of all vesicles, regardless of number of DNA oligos, occurred at a 50 mM salt concentration.

(63) INVESTIGATION OF TETHERED PHOSPHOLIPID VESICLE ASSEMBLIES USING QUARTZ CRYSTAL MICROBALANCE WITH DISSIPATION AND FLUORESCENCE MICROSCOPY
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The realization of a robust, fluid, defect-free cell membrane model, able to house a variety of functional integral proteins, has been elusive despite abundant attention by numerous groups. We have constructed a tethered phospholipid vesicle assembly via a biotin-streptavidin linkage that has the potential to overcome the major limitations of other model membrane environments: protein-substrate interactions in planar supported bilayers; and dewetting, low fluidity, and defects present in many polymer-supported bilayer membranes. Using quartz crystal microbalance with dissipation measurement (QCM-D) and fluorescence microscopy, we demonstrate the construction of a molecular assembly in which liposomes are specifically tethered to a planar supported lipid bilayer. We are able to monitor the step-by-step formation of the assembly in addition to being able to measure differences in frequency and dissipation data corresponding to differently sized vesicles. During the course of this investigation, we have discovered a biotin-mediated membrane-membrane interaction and have also been able to measure water content in a streptavidin monolayer.
(64) ADHESION OF FUNCTIONALIZED PARTICLES TO TETHERED LIGANDS UNDER SHEAR FLOW
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The architectural effects of ligand-bearing tethers on their binding to model receptor surfaces was studied using a flow cell. Specifically biotin ligands were stationed to a bilayer coated surface through end-grafted polymer chains and the receptors were free flowing streptavidin coated microspheres with a size of either two microns (fluorescent) or six microns (non-fluorescent). Varying amounts of lipid-PEG and lipid-PEG-biotin were deposited onto glass slides hydrophobized by octadecyltrichlorosilane (OTS) using a Langmuir Blodgett trough. The strength of the ligand-receptor bond was investigated by varying shear rates. The attachment and detachment rate was also explored by fluctuating the shear rate. Fluorescence microscopy was used to compare the number of particles bound to each architecture.