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**AFM-IR study to understand the microstructure and chemical composition of Type I collagen fibrils for estrogen depleted and drug treated lumbar vertebrae**

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Over 75 million people in the world suffer from the bone disease osteoporosis. Type I Collagen is an important structural component that contributes to the mechanical properties of bone such as toughness. It is known that estrogen depletion and drug treatments alter the microstructure of Type I collagen. However, the basis of the changes is not well understood. Traditional AFM technique only provides morphological information. With the AFM-IR technique, fibril topography and chemical composition, from the infrared spectrum, of collagen fibrils can be simultaneously obtained. Four sets of lumbar vertebrae sections (sham, estrogen deficient (OVX), OVX plus a cathepsin-K inhibitor, and OVX plus alendronate) after 24-months of treatment are examined with AFM-IR to evaluate how long-term treatment effects of the two bone resorption inhibitors on the microstructure of Type I collagen and the chemical origin of the microstructural changes of Type I collagen within the trabecular region of lumbar spine.
Cloisite 30B as Nanoclay Compatibilizer for Polysulfone/Polyimide Blend Films

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ABSTRACT:

Polysulfone (PSF) and polyimide (PI) are used in many applications including membranes for gas separation and water purification. The phase separation issues limit the blend application of these polymers. We studied the effect of nanoclay and Cloisite 30B had on (PSF/PI) films. This was done in order to examine the compatibility effects of clay on phase separation behavior, mechanical strength, and structure properties. The addition of weight percentage of organoclay strongly compatibilized the blend phases for all compositions, decreasing the scale of blend phase separation by a factor of 5-10. Interestingly, the net phase separated domain area converged to the 50% blend composition in all cases. This is attributed to a high degree of exfoliation and degradation of nanoclay particles within the PSF/PI matrix as well as interfacial regions, independent of the blend composition. AFM confirmed these optically observed compatibilization effects by quantitative reduction of aspect ratio (width/height) of surface phase separated domains. As a consequence, the mechanical properties have improved slightly by adding C30B particles. This has been represented in our study by an increase in tensile modulus. However, further increase in nanoclay loading decreased the tensile strength and elongation at break. The surface free energies of the films decreased by adding C30B. This has lead us to conclude that there is a changing of surface topography, which conformed to the contact angle. TGA measurements of PSF/PI films showed decreasing in thermal stability by adding C30B due to the surfactant modification of C30B.
Novel Detection of Surface Enrichment Driven by Molecular Weight Disparity in Polymers

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The segregation of one component of a polymer blend to its surface is important to the ultimate performance of devices fabricated from polymeric materials, and improved methods for elucidating such segregation will allow advances in many applications such as adhesives, coatings, membranes, and biomaterials. Of particular interest is surface segregation that leads to formation of a complex single phase containing a concentration gradient rather than macroscopically phase separated layers. This surface segregation can allow for surface properties that differ from the bulk without the loss of mechanical strength that accompanies phase separation.

It has been seen in the past that differences in the molecular weight of macromolecules can drive surface enrichment, due to entropic contributions of end groups. This work demonstrates the ability of an emerging analytical technique to detect enrichment that cannot be observed with any other technique, and can elucidate the degree of enrichment with unparalleled precision. Using polystyrene and polymethyl methacrylate ranging from 2000 Da to 17000 Da with a polydispersity less than 1.05, enrichment of chains differing by less than 300 Da (~3 repeat units) is observed on the surface of thin films of these materials. This is unprecedented given the lack of diversity in chain length in these distributions.
Development of Polymeric SO₂ Resistant Coating for Solid Amine Sorbent

Hailiang Jin

ABSTRACT

The impurities in flue gas from coal fire power plant such as SO₂, could poison CO₂ sorbent due to its strong acidity. To reinforce the stability of sorbent in presence of SO₂, polymeric SO₂-resistant coating was developed and characterized by in-situ FTIR spectroscopy. This coating was prepared by crosslinking tetraethylenepentamine (TEPA) with an epoxy and applied to CQA-12, a solid amine sorbent. The effect of the epoxy composition on the stability and adsorption / desorption kinetics of the coated sorbent was investigated by FTIR and mass spectrometry. The results revealed that this polymeric coating enhanced the resistance to SO₂ poisoning, thus the multi-cyclic stability of the sorbent in presence of SO₂, by converting the amine sites to secondary and tertiary amine. Though it reduced the initial CO₂ capture capacity due to blocked amine sites. Increased amount of epoxy was found to strengthen the SO₂ resistance. The FTIR spectra denoted that the introduction of epoxy increased the ratio of weakly adsorbed CO₂ to strongly adsorbed CO₂, i.e., reduced the binding strength of amine/CO₂.
Model compound study to characterize the development of Acetoacetate functionalized resin derived from Kraft lignin.

By: Eric M. Krall, Dean C. Webster

Developing new carbon based materials from terrestrial carbon sources instead of fossilized carbon will help reduce humanity’s dependence on petrochemicals. Lignin provides a viable source of terrestrial carbon with unique chemical properties. Kraft lignin is currently a byproduct of the paper pulping industry which makes it an excellent candidate for development into value added chemicals. This research is focused on turning Kraft lignin into a functionalized resin open to a variety of crosslinking mechanisms. Acetoacetate functional groups can readily react with melamine, amine, aldehydes and acrylate groups which will lead to the development of a variety of new thermosetting polymers. In order to characterize the degree of acetoacetate functionalization this study uses a model compound characterized by NMR and Mass Spectrometry techniques to aid in the understanding of how different hydroxyl environments are functionalized with acetoacetate groups.
Nanoporous membranes have been studied for several years for the separation of oil-water mixtures. In our work, rather than focusing on aqueous phase purification, we are designing membranes that are intended to interact with the organic compounds. These membranes are fabricated from self-assembling poly(methyl methacrylate-\textit{b}-(dimethylsiloxane-\textit{co}-vinylmethylsiloxane)) block copolymers. In order to enhance fluid transport through the membrane, the cylinder nanostructure morphology is targeted, and the nanoporous membrane is aligned parallel to the direction of flow via solvent annealing. Following alignment, exposure to UV light cross-links the siloxane copolymer block to impart mechanical integrity and degrades the sacrificial PMMA block in a single step. Future work measuring oil flux and membrane swelling will assist in further understanding the transport capabilities of hydrophobic species through the membrane with high selectivity and mechanical integrity being desired. In addition to the membrane work, complementary studies on the effect of BCP architecture (topology) on self-assembly of thin film (thicknesses ~10-100 nm) will be presented. This work focuses on unique properties that nonlinear architectures (cyclic and star) offer in comparison to linear poly(styrene-\textit{b}-methyl methacrylate). For example, cyclic BCPs self-assemble with smaller domain sizes than their linear counterparts, and the entropic contributions to the self-assembly of star BCPs may assist with nanostructure alignment.
Post-synthetic Polymerization of Porous Organic Materials for Gas-Separation Membranes

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Abstract: Improving the efficiency of membrane-based gas separations remains a formidable challenge owing to the compromise between attaining high selectivity and high permeability; thus, further research is required to fully realize the potential of these materials to displace conventional gas separation approaches. Although there have been a range of studies on metal-organic framework (MOF)-based membranes, there is currently a dearth of studies on membranes based on porous organic materials such as covalent-organic frameworks (COFs) and polymers of intrinsic microporosity (PIMs), despite their several advantages.

In this project, COF and PIM particles were synthesized via imine condensation and copper (I)-catalyzed azide–alkyne cycloaddition (CuAAC) polymerization reactions, respectively, from tetrahedral monomers. The resultant porous organic particles were characterized using nitrogen adsorption/desorption isotherms, scanning electron microscopy, and X-ray diffraction to determine surface area, porosity, and particle size, and the characteristics of the crystalline COF particles were compared to the amorphous PIM particles to demonstrate the role of crystallinity. The crystalline COF particles were then surface functionalized and copolymerized with methacrylate monomers to obtain thin films, and the gas separation properties of the attained films were characterized.
Automated Image Analysis Quantifies Orientational Order in Polymer Nanofiber-based Thin Film Transistors

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A comprehensive image analysis framework is introduced to quantify the shear-induced alignment of poly (3-hexylthiophene) (P3HT) nanofibers and its impact on charge transport in polymeric transistors. Bottom gate, bottom contact organic field effect transistors were fabricated from a solution of P3HT in chloroform that was sonicated and aged for up to eight days. The active layer meso-scale structure was characterized by collecting three 10 x 10 \( \mu \text{m} \) atomic force microscopy images directly from within the device channel. The image analysis procedure utilizes coherence-enhancing anisotropic diffusion filtering, thresholding, and skeletonization to extract fiber orientation distributions and the frame-size-dependent 2-dimensional order parameter, \( S_{2D} \), for each device. Field effect hole mobility is found to be linearly correlated with \( S_{2D} \) over length scales from 4 – 10 \( \mu \text{m} \). This correlation is demonstrated for fibrillar structures near the dielectric interface of high performance devices (mobility > 0.1 cm\(^2\) V\(^{-1}\) s\(^{-1}\)), and is shown to be valid for individual devices, resolving performance differences that arise from structural variance developed during thin film deposition. The trend in mobility is attributed to the improved grain boundary structure induced by the presence of large aligned domains of nanofibers. A study of the morphological impact of spin-coating using the same image analysis procedure demonstrates that fiber orientation and alignment are strong functions of the spin-coating flow field, with orientation displaying a significant radial bias and alignment increasing with distance from the center of spin coating. The results demonstrate the utility of image quantification for constructing process-structure-property relationships, while showing that a rapid, high-shear deposition method can be used to induce the structural order necessary to obtain high performance polymeric transistors.
Chemical Oxidation of Soluble Electroactive Polymers: A Route Towards Scalable Device Construction

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Conjugated polymers are used as active materials in electrochemical applications such as supercapacitors and electrochromic devices (ECDs). Our group has developed an extensive family of soluble dioxothiophene-based polymers (PXDOT) to suit both of these applications. For ease of synthesis and purification, all of the polymers are synthesized in their charge neutral form. However, in order for supercapacitors to reach full depth of discharge and for ECDs to reach full contrast immediately after device assembly, the two electrodes should be in different oxidation states. This is typically done by electrochemical oxidation/reduction prior to device assembly; however, that method is not adaptable to roll-to-roll manufacturing.

Here, we evaluate the use of chemical oxidation as a more scalable and efficient alternative to electrochemical oxidation. This can be performed either by dipping the films in an oxidant solution or casting films from co-dissolved polymer and oxidant solutions. We will discuss how the extent of oxidation can be manipulated by varying time, concentration and oxidant species. We will also show that this chemical oxidation step/co-processing can be done in ambient conditions and that it has no effect on the extent of polymer oxidation. As a proof of principle, we have assembled ECDs that have a chemically oxidized charge storage polymer as the counter electrode. These devices achieve full contrast immediately after assembly confirming that this approach is a promising route towards high-throughput manufacturing of ECDs and other polymer-based electrochemical devices.

Identifying Kinetic and Thermodynamic Effects on
Self-Stratifying Polymer Blends

Samantha Rinehart
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Coatings are used on everyday surfaces for protection and to improve durability. An intriguing development of the coating industry, whether used for outer-protection of cars or other layered surfaces, is the self-stratification of multi-component systems. The self-assembly properties of polymers present an attractive avenue for thin film deposition. The morphologies formed by self-stratification can be altered simply by modifying processing conditions. However, current use of self-stratification utilizes polymer blends specific for the desired application and does not take into consideration the entire process of stratification. Understanding the role of kinetic and thermodynamic effects on the final polymer depth profile formed by self-stratification is fundamental in improving the ability to apply self-stratification to a wide array of systems and applications. The current research investigates the self-stratification during spin-coating of polymer blends by combining three themes: understanding solution phase behavior, monitoring film formation in-situ, and determining the depth profiles of the final film. These three themes will provide insight into the main driving force that govern the self-stratification of polymers. This research has potential to impact a wide range of technologies ranging from organic electronics to the coating industry by developing a cost efficient method for multi-layer film deposition.
Highly Functional Methacrylated Bio-based Resin System for UV-Curable Coatings

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Methacrylated epoxidized sucrose soyate (MESS) was synthesized from epoxidized sucrose soyate (ESS) and methacrylic acid, producing a highly viscous bio-based resin. Because of this, styrene was used as a reactive diluent to lower its viscosity. MESS was characterized using Fourier transform infrared spectroscopy (FTIR), proton nuclear magnetic resonance spectroscopy ($^1$H-NMR), gel permeation chromatography (GPC), and viscosity measurements. Various formulations containing styrene were used to produce thermally initiated, free-radically cured, bio-based thermosets with high glass transition temperature with good mechanical properties. The versatility of this resin was explored and applied in UV-cured coatings for dental composite applications. This resin was combined with various di- and trimethacrylated reactive diluents and cured using a photoinitiator (Irgacure 1173) at a 4:1:0.25 ratio, respectively. The extent of cure was determined by % gel content using Soxhlet extraction and confirmed using FTIR. The thermal and mechanical properties were determined by thermogravimetric analysis (TGA), dynamic mechanical thermal analysis (DMTA), and tensile testing. Coatings made from these formulations displayed good solvent resistance and hardness due to the high crosslinking. Consequently, the coatings were very brittle and inelastic, shattering easily when subjected to impact testing and Mandrel bending. Commercially available Bisphenol A glycerolate dimethacrylate (BisGMA) was used as the control.
Thermal Conductivity of PEEK/BN Composites in an Injection Molded Process

Glenn Spiering
Anne Musgrave
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Abstract
Composites of poly(etheretherketone) (PEEK) and boron nitride (BN) have been tested to determine their thermal conductivity. BN is a ceramic with high thermal conductivity, and PEEK is a thermoplastic that demonstrates common polymer insulating properties. A silane coupling agent was introduced to improve the bond between the PEEK and BN. Multiple loading levels of the BN were studies to determine the effects the amount filler has on composite thermal conductivity. Samples were prepared by twin screw extrusion compounding followed by injection molding, resulting in BN particles aligned in the direction of the polymer flow. Thermal conductivity both parallel and perpendicular to filler orientation were tested to analyze directional effects caused by molding orientation. Perpendicular to the orientation of the BN filler, the composite exhibited little change in thermal conductivity with increasing BN loading. Increases in the filler loading increased the thermal conductivity of the composite in the orientation parallel to the BN filler up to 1200% at the maximum filler loading level of 40% BN by mass.
Thermotropic Telechelic Ionomers for High Performance Applications

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Thermotropic liquid crystalline polymers are most notable as a result of their anisotropic behavior above the melting point of the material. Rigid rod like monomers result in polymers with high chemical and thermal resistance. The rigid behavior of these polymers have the enhanced benefit of significant shear thinning, which is advantageous to injection molding of small electronic parts. The downfall of traditional LCPs is owed to the brittleness and difficult high temperature synthesis that often involves a secondary solid-state polymerization step. A variety of methods have been attempted to improve upon these deficits, including the addition of post polymerization chemical or physical crosslinking. Incorporation of ionic charge groups into polymers has shown to create a physical crosslinked network that can improve mechanical properties of semi-crystalline polyesters. This work describes the synthesis and characterization of oligomeric telechelic ionomers to create polymers with a well-controlled charge location that may result in easier processing and improved mechanical properties over their high molecular weight counter parts. A series of PET-ionomers with the sodium 3-sulfobenzoate monofunctional endcapper were polymerized using melt transesterification. This standard created telechelic ionomers with a series of molecular weights from 4000-30,000 g/mol, confirmed by $^1$H NMR. Thermal and rheological characterization was performed to understand the combined effects of molecular weight and % ionic aggregation. Work has begun on monofunctional ionomer incorporation into a well-studied LCP, poly(hexamethylene-4,4’-bibenzoate). This area will focus on understanding the effect of the ionic group incorporation and molecular weight on the crystallinity and mechanical properties of LCPs.
Title: In-situ Mechanistic Investigation of an Organic Radical Polymer Cathode on Interfacial Charge and Mass Transfer

Authors: Shaoyang Wang, Fei Li and Jodie L. Lutkenhaus

Organic radical polymers have gained increased attention as cathodes for organic radical batteries (ORBs) due to their fast charge transport and high cycling stability. These features make them a promising alternative to conventional lithium-ion batteries. One polymer of interest is a nitroxide radical polymer, poly(2,2,6,6-tetramethylpiperidinyloxymethacrylate) (PTMA), which is capable of a two-electron transfer process. PTMA as a cathode has a reported specific capacity between 77 to 220 mAh/g, depending on the charge/discharge conditions. Most work with PTMA has largely emphasized electrode optimization to improve its capacity by adding highly conductive materials or by designing new forms of radical polymers. There is little molecular level detail on the charge storage process and the electrode/electrolyte interface in such systems. Here, we present the application of in situ electrochemical quartz crystal microbalance with dissipation monitoring (EQCM-D) towards the charge storage process in PTMA. EQCM-D monitors various electrode physical properties (e.g. mass, shear viscosity) during controlled electrochemical interrogation (cyclic voltammetry). Preliminary data suggests EQCM-D is able to provide insight in depth on such interfacial charge transport phenomenon.
Synthesis, modification and characterization of the amine cured epoxy films

Author: Sihan Wang

Novel films of epoxy and amine was synthesized and has the applications in the field of CO\textsubscript{2} separation / adsorption. In this study, the amine functionalized epoxy films were made for CO\textsubscript{2} separation films and also the pelletization of the solid amine CO\textsubscript{2} capture sorbents. The amine-epoxy films was also modified by silica nanoparticles as the mechanical reinforcement agent. The synthesis process and were characterized by FTIR and Raman spectroscopy. The physical properties of the film were studied by SEM, TEM, TGA and DSC. The interphase properties of the film with gas phase CO\textsubscript{2} were characterized by in situ FTIR and mass spectrometry.
Title: Polymerization of silyl ketenes

Institute name: Case Western Reserve University

Author: Yuanhui Xiang

Abstract: Development of unique polymeric backbones and structures is key to accessing novel materials and expanding the usefulness and applications of polymeric materials. Herein we report experimental and theoretical investigations of the polymerization of triisopropyl silyl ketene using alkoxide initiators, and identify the oligomeric and polymeric products formed. Triisopropyl (TIPS) ketene reacts with benzyl alkoxide to give a delocalized anion that can polymerize through the oxygen or carbon atoms to give polyacetal and polyketone, respectively. This work gives insight into the design of new monomers and lays a foundation for the preparation of multiple polymer backbone functionalities from a single monomer.
Influence of Ions on Diffusion of Water at the Metal/Coating Interface

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Abstract

The evaluation of the anti-corrosion properties of coatings are mostly based on the macroscopic corrosion phenomena. While empirical knowledge of effective corrosion mitigation strategies is available, a fundamental understanding on the nanoscale of the corrosion at the coating/metal interface is lacking. Additionally, an evaluation of interface reliability based on a fundamental understanding of the corrosion process between the metal and coating at very short times and on the nanoscale could speed coating evaluation. The objective of this work is to study water movement at the coating/metal interface at short times and nanoscale to infer long time behavior and elucidate how water reaches corrosion sites away from coating defects. X-ray reflectometry (XR) and Neutron Reflectometry (NR) were used. NR was used to nondestructively determine the depth profile of a substance near an interface with a resolution of 1-2 nm\textsuperscript{1}. The diffusion of water at the coating/oxide interface was evaluated with and without the influence of ions. Results from XR and NR were also compared with electrochemical impedance spectroscopy (EIS) measurements\textsuperscript{2}, which are widely used in the evaluation of anticorrosion properties of coatings.

References:


Diketopyrrolopyrrole-Based Oligophenylenethiophenes with Latent Hydrogen Bonding for Solution-Processed Organic Field-Effect Transistors

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Abstract
Two diketopyrrolopyrrole (DPP)-based oligomers with phenylene/thiophene moieties and a thermal liable 2-methylhexyl-2-oxylcarbonyl (mHoc) group, mHocPBT and mHocTBT, were synthesized and used for solution-processed organic field-effect transistors. The oligomers can be readily dissolved in common organic solvents and further converted to strong intermolecular hydrogen-bonded, pigment-like materials by thermal annealing the casted solid film at a temperature between 180 and 200 °C. Effects of the activation of latent hydrogen-bonding networks on the properties of oligomer films, including UV/Vis absorption spectra, band gap, solvent resistance, film morphology, molecular packing mode, and charge mobility are investigated. Highly crystalline films and significantly improved field-effect mobility of the device was observed on mHocTBT oligomer after annealing treatment, suggesting an efficient control of molecular packing, film morphology and device performance of the latent hydrogen-bonding strategy.
Figure (If needed)

[Diagram showing polymer characterization process]

D-A system
Enhanced Solubility and Solution Processability

Heat

Intermolecular Hydrogen-Bonding Network

$t$-Boc Protected Latent Pigment
$m$-Hoc Protected Latent Pigment

$\text{Latam-triiod Conjugated Structure}$
$\text{Chain Extended}$
$\text{Latam-triiod Conjugated Structure}$
$\text{Thermal Activation}$
$\text{Latam-triiod Conjugated Structure}$

$\text{mHocPBT}$
$\text{mHocTBT}$

$\text{CO}_2$ (b.p. 92 °C)
Photocatalytic Reduction of CO$_2$ by PEI Functionalized TiO$_2$ Thin Film

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Photocatalytic reduction of CO$_2$ is considered as an integral part of an energy storage strategy to store energy in the formation of hydrocarbons fuels. TiO$_2$ based photocatalyst has attracted the most attention due to its excellent stability, nontoxicity as well as cost-efficiency. However, the photocatalytic reduction of CO$_2$ by TiO$_2$ based catalyst is hampered by its low reduction efficiency, which primarily attributes to the rapid recombination of photo-generated electron / hole pairs and the low affinity of CO$_2$ toward to TiO$_2$ surface. Application of voltage onto photocatalytic process can create an external electrical field suppressing the recombination of electron / hole pairs.

In this work, we investigated the feasibility of employing a polyethyleneimine (PEI) functionalized TiO$_2$ to capture and photocatalytic reduction of CO$_2$ into hydrocarbon fuels. The nature of CO$_2$ adsorption and photocatalytic reduction process were studied by in situ infrared spectroscopy coupled with mass spectrometer. The results showed that PEI-TiO$_2$ performs excellent CO$_2$ capture ability and CO$_2$ rapidly adsorbs on PEI-TiO$_2$ as the form of carbamate, ammonium ions. Photocatalytic reduction of CO$_2$ was examined as CO$_2$ or CO$_2$/H$_2$O adsorbed on PEI-TiO$_2$. The adsorbed CO$_2$ species can be photo-reduced to formate species by irradiating with UV under 1 volt of voltage applied, which is evidenced by the formation of IR band at 1692 cm$^{-1}$. PEI-TiO$_2$ exhibits higher photo-reduction efficiency with CO$_2$/H$_2$O adsorbed compared to with only CO$_2$ adsorbed. The analysis of gaseous reduced products showed that adsorbed CO$_2$ was reduced to formic acid, ethane and ethanol. Photo-generated current can be detected in this process and presence of H$_2$O accelerated the utilization of photo-generated electrons resulting in lower level of current.
Molecular Design, Synthesis and Characterization of p- and n-Channel π-Conjugated Donor-Acceptor co-Polymers and Applications in Thin Film Devices

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Polymeric semiconducting materials possessing effective $\pi-\pi$ intermolecular interactions coupled with good solution processability have been highly investigated. 2,2'-bithiazole was copolymerized with dithienyldiketopyrrolopyrrole to afford a novel n-channel poly(dithienyldiketopyrrolopyrrole-bithiazole), PDBTz. PDBTz exhibited pure n-channel behavior with excellent ambient stability and an electron mobility reaching \(0.3 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}\) based on organic field-effect transistor (OFET) characterization, in contrast to a recently discussed isosteric conjugated polymer, a copolymer of the electron rich bithiophene with dithienyldiketopyrrolopyrrole possessing pure hole transport (p-channel) characteristics. This inversion of charge carrier transport characteristics suggests a significant potential for bithiazole in developing robust n-channel semiconducting materials. Significantly, 5-DH side-chain was incorporated into PDBTz to enhance polymer solubility in non-halogenated solvents, and hence the system may have desirable characteristics for large-scale fabrication of devices. PDBTz cast from non-halogenated solvents exhibited excellent electron transport performance based on OFET results, and film morphologies commensurate with high mobility.

While the previously reported pTBTD-5DH material exhibits superior qualities with respect to the degree of polymerization, solution processability, $\pi-\pi$ interchain stacking, and charge carrier transport properties (hole mobility of as high as \(2.95 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}\)), its n-type analog exhibits a lower charge carrier mobility. However, with various processing techniques, it is believed that the carrier mobility can achieve higher levels. This leads ways to applications, such as P-N complementary circuits, thermoelectric devices, all-polymer solar cells etc.
Synthesis, Characterization and Application of Porous Polymer Thin Films and Particles

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Porous polymer materials have attracted increasing interest because of their extraordinary properties and functionalities which could be effectively applied in adsorption area. This presentation will include development of environmental-benign materials, porous polyvinyl alcohol (PVA) supports and their functionalization with polyamines, for CO$_2$ separation / adsorption from power plant and dye removal from waste water. The porous PVA thin films and particles were synthesized via phase inversion method and crosslinked with di-functional molecules in a systematical study. The support was then functionalized with polyamines and crosslinkers in order to create an insoluble network. The physical properties of materials were characterized by SEM, TEM, TGA and BET. The interfacial properties of polyamine-functionalized porous PVA materials with gas phase CO$_2$ were studied by transient infrared spectroscopy.
Improving performance of organic solar cell using sequence effect

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Sequence is recognized as a versatile and efficient structural tool to tune properties of biopolymers and increasingly in synthetic polymers. Polymer degradation, crystallinity and self-assembly behaviors have all been shown to depend on monomer sequence. Despite these findings there has been little effort directed at exploring the effects of sequence in conjugated materials. In a previous study, we demonstrated that changing the sequence of substituted and unsubstituted phenylene vinylene units in oligomers the electrochemical band gap could be shifted over a 0.24 V range. In the current study, we extend the research to donor-acceptor type oligomers and polymers comprising benzothiadiazole and phenylene vinylenes units. The effect of monomer order on the electrochemical and optical properties of these materials will be reported as will the results of simulations of these materials using density functional theory calculations. The effect of sequence on the performance of these materials in devices will also be discussed.