The Effect of Annealing Temperature and Time on the Crystallinity of Poly(Lactic Acid)
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Poly(Lactic Acid) is a thermoplastic polymer and derived from renewable sources such as cornstarch. PLA biodegrades after use, if composted. The purpose of this project is to investigate the effects of annealing temperature and time on the crystallinity and crystalline structure of Poly(Lactic Acid) using differential scanning calorimetry (DSC), wide angle x-ray diffraction (WAXD), and dielectric relaxation spectroscopy (DRS).

Cross-linking of Hydroxyl Functionalized Polypropylene for Capacitor Applications
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Capacitors represent one of the most commonly used energy storage devices. Industrial impetus always exists to improve current devices in a commercially viable fashion. The energy density \( J \) of a plate capacitor is governed by the dielectric constant \( \varepsilon \) and breakdown strength \( E \) of the insulating media through a simple equation: \( J = \frac{1}{2} \varepsilon \varepsilon_0 E^2 \). Previous studies indicate that functionalization of polypropylene (PP) with polar hydroxyl side groups increases dielectric constant (2) and that cross-linking PP can increase breakdown strength.
**Fluorescence Quenching of Donor/Acceptor Mixtures for Organic Solar Cells**

*REU Student: Edmund Burnett, Department of Chemical and Bimolecular Engineering, Clarkson University*

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P3HT/PCBM is the most commonly used mixture for the active layer in organic solar cells. However, more in depth research is necessary to characterize the effectiveness of the mixture. Fluorescence spectroscopy is used to evaluate charge transport between P3HT to the receiving species. X-ray diffraction was also used to further understand what qualities of the mixture affect the difference in fluorescence quenching and thus charge transference.

**Mechanical Testing of Ion-Containing Polymers**

*REU Student: Julianne Carlson, Department of Materials Science and Engineering, Pennsylvania State University*

*Graduate mentor: Melanie Disabb-Miller*

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The attractive properties of ion-containing polymer films have lead to an increase in demand of these membranes, specifically for use in fuel cell applications. To have a mechanically robust material that will last a long time in a working device, it is important to understand how the backbone composition and water uptake properties of specific polymers influence their mechanical properties.

**Mechanical Testing of Ion-Containing Polymers**

*REU Student: Proma Debnath, Department of BioEngineering, Pennsylvania State University*

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Biomaterials are nonviable materials used in medical devices, intended to interact with biological systems. The goal is formulation of structure property relationships that relate material surface energy to the biological response to these materials when implanted into different physiological compartments. This will enable prospective design and optimization of biomaterials.
OMIM Geometry and Microporous Behavior
REU Student: Ben M. deGlee, Department of Materials Science and Engineering, University of Florida
Graduate mentor: Lauren Abbott
Faculty Advisor: Coray Colina
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There is increasing interest in Materials exhibiting Intrinsic Microporosity (IM), defined as having pore sizes below 2nm resulting from the inherent molecular structure of the substance. The extremely high surface area density of these materials allows for a maximization of surface interactions; therefore, they show great potential in applications such as gas storage, separation, and catalysis. Here we study Organic Molecules of Intrinsic Microporosity (OMIMs), large molecules with rigid and concave structures that inefficiently pack to form amorphous Microporous materials.

How Plasticizers Enhance Ion Conduction in Ion-containing Polymers
REU Student: Patrick Dixon, Materials Science and Engineering, Georgia Tech University
Graduate mentor: U Hyeok Choi
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Many batteries, which power contemporary mobile electronic devices, rely on ion-containing polymers to serve as electrolytes. However, generally ion-containing polymers require the addition of plasticizers, to increase their conductivities to useful values. The goal of this study is to determine the mechanisms by which plasticizers increase the conductivities of ion-containing polymers.
Thermal Behaviour of Poly(p-dioxanone) Rings

REU Student: Yuedan Dong, Department of Chemical Engineering, Pennsylvania State University
Graduate mentor: Helen Wang
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Poly(p-dioxanone)( PPDO) is getting a lot of public attention in medical industry from 1980s. PPDO is aliphatic polyetherester with excellent flexibility and biodegradability. It is absorbable polymer, which has widely application in medical industry, like bone or tissue fixation devices and drug delivery systems. The purpose of this project is to investigate the thermal behavior of Poly(pdioxanone) rings used for biodegradable implants in heart that hold arteries open for about 8 months.

Water Wetting of Biomaterials and the Goldilocks Surface

REU Student: Michael Fortunato, Department of Materials Science and Engineering, Pennsylvania State University
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Biomaterials research is aimed at discovering materials for use in biomedical devices. Biocompatibility is determined by how well a device meets the requirement of end use, measured by the intensity of the biological response to the surface material. Two types of biological responses have previously been observed. The intensity of type I biological responses (e.g. protein adsorption) decreases with increasing hydrophilicity, while the intensity of type II biological responses (e.g. blood plasma coagulation) decreases with increasing hydrophobicity. Between I and II is a minimum in the biological response and presumably a maximum in biocompatibility...The Goldilocks Surface.

The Separation Of Hydrocarbons From Sand Using Ionic Liquids

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To apply a new, unique method of separating bitumen from tar sands using environmentally friendly ionic liquids. Initially imidazolium based ionic liquids (ILs) were used, however the focus turned to third generation ILs, which are stable, inexpensive, and environmentally friendly ILs consist of large organic cations associated with various anions Most melt at or below 100°C with negligible vapor pressures Many ILs are liquids at room temperature and have outstanding chemical and thermal stability

Amorphous Linear Polymers : Verification by Simulation
REU Student: Grant Gonzalez, School of Engineering and Applied Sciences, Harvard University
Graduate mentor: Lauren Abbott
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Simulation methods have been devolved to study complex, large and bulky amorphous polymers. For the first time, this simulation methodology will be extended and verified for various amorphous, linear polymers. The following four polymers though differing in backbone rigidity and complexity will be simulated by the same methodology.

Evaluation of Colloidal Properties of Submicron and Nanoscale Diamond for Structural Applications
REU Student: Michael Haider, Department of Materials Science and Engineering, Rowan University
Graduate mentor: BL Babcox
Faculty Advisor: James Adair
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Investigate colloidal properties of diamond suspensions. Minimize size of as-received colloidal particles. Create diamond slurry for fabrication of porous diamond parts.

**Resonance Raman Simulations of Carbonmonoxy Myoglobin: A QM/MM Study**

*REU Student: Benjamin Holt, Department of Chemistry and Department of Mathematics, Wofford College*

*Graduate mentor: Daniel Silverstein*

*Faculty Advisor: Lasse Jensen*

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The goal of this project was to create simulated resonance Raman spectra of a large protein that are comparable to experimentally obtained spectra by utilizing hybrid QM/MM calculations. This required understanding of Density Functional Theory (DFT) calculations, simulation parameters, and how electronic structures relate to both DFT and Resonance Raman.

**Conductivity and Water Uptake of Proton Exchange Membranes for Fuel Cells**

*REU Student: Zach Johnson, Department of Materials Science and Engineering, Pennsylvania State University*

*Graduate mentor: Melanie Disabb-Miller*

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Fuel cells are becoming increasingly important for renewable energy applications. My research focuses specifically on the polymers in proton exchange membrane fuel cells. To determine the differences between random and block copolymers, I examined their water uptake, ion conductivity, and ion exchange capacity (IEC). IEC is polymer characteristic that describes the number of ions per mass and can help to predict a polymer’s potential as a fuel cell membrane.

**How Phosphonium-based Ionic Liquid Counterions Govern Ionic Conductivity of Polymer-sulfonate Ionomers**

*REU Student: Quang Ly, Department of Chemical and Biomolecular Engineering, North Carolina State University*

*Graduate mentor: Gregory J. Tudryn*

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Improvements in polymer electrolyte systems play an integral part in energy storage applications. Poly (ethylene-oxide) (PEO) based polymer electrolytes with a dissolved lithium salt have been the mainstream research focus due to the ability of ether-oxygen to disrupt salt aggregates and solvate Li+. Ionomers are polymers with tethered charges which govern bulk properties by the ionic interactions in discrete regions of high polarity, known as ionic aggregates. These systems often have limited conductivity due to strong ionic interactions and aggregate formation. We utilize ionic liquid counterions to weaken ion pair interactions. The use of bulky counterions plasticize and disrupts ion associations (aggregation) without additional solvent, thus improving conducting ion density and ion mobility in ionomers used for electroactive devices. Phosphonium-based ionic liquid counterions are of interest in place of ammonium-based ionic liquid counterions1 because they offer favorable charge delocalization, promising better conducting ion density, and thus higher conductivity.

**Diffusion and Solubility of 1-Octene in Polyethylene via Gravimetric Sorption**

**REU Student:** Changjian Ma, Department of Chemical Engineering, Pennsylvania State University  
**Faculty Advisor:** Ronald Danner  
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Why study diffusion and solubility of 1-octene in polyethylene? Polyethylene is used in many products, 1-octene is a typical solvent to make branched polyethylene, 1-octene can be health or safety hazardous.

**DFT methods to calculate pairing energies between sulfonate and quaternary ammonium quadrupoles**

**REU Student:** Ernesto Martinez, Department of Materials Science, Massachusetts Institute of Technology  
**Graduate mentor:** Ping Lin  
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Ion-containing polymers behave differently than neutral polymers due to the strong ionic interaction between charged monomers. Charged species often assemble into electric quadrupoles such as:
These ionic interactions between monomers can influence the radius of gyration of the polymer due to the strong ionic interactions compared to Van der Waals forces or hydrogen bonding interactions in other types of polymers. Dimerization free energies can be calculated for these quadrupoles to determine exactly which species will interact most strongly. Dimerization Energy is calculated by the following equation: Dimerization Energy = Dimer Energy – 2 x Monomer Energy These energies were calculated using advanced \textit{ab initio} quantum mechanical methods. Calculating the energies of these molecular systems involves finding an approximate solution to the time-independent Schrödinger Equation: \[ \mathcal{H}(\mathbf{r}) = E \Psi(\mathbf{r}) \] where \( \mathcal{H} \) is the Hamiltonian operator, \( E \) is the energy of the particle and \( \Psi \) is the wavefunction. Density Functional Theory (DFT) allows for approximate solutions to the Schrödinger Equation. The main principle of DFT is that the total electronic energy and other molecular properties are related to the overall electronic density of the system. Thus \( E \) is a functional of the function \( \rho(\mathbf{r}) \), the density function. DFT is often the preferred method for computing these energies as it takes into account the electronic correlation from the start, as opposed to other methods. However, the Hartree-Fock theory provides an exact method for taking into account the exchange contribution. This lead for an HF/DFT hybrid method to be used called B3LYP, which uses exact exchange energies from HF and corrected correlation energies from DFT. To solve these equations an initial guess to the density is used from which a set of orbitals is obtained that in turn leads to a refined value for the density, which is used again in the same fashion, until it converges. This approach is said to be self-consistent.

**Viscoelastic behavior of Bovine Serum Albumin in Solution**  
*REU Student: Joel Millan, Department of Chemistry, University of Puerto Rico-Humacao*  
*Graduate mentor: Maria-Monica Castellanos*  
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The rheological behavior of protein solutions are of interest to the pharmaceutical and medical communities, as their response affects their processing and functionality. Protein solutions exhibit a shear thinning response when subject to a steady shear showing high viscosities at low deformation rates. A rheopectic behavior is believed to be due to the formation of aggregates that leads to an unexpected increase of the viscosity at different conditions of concentration, ionic strength, temperature and pH.

Bovine serum albumin (BSA) is one of the most widely studied globular proteins, because of its availability, biological relevance (i.e. blood, synovial fluid) and similarities with the analog human serum albumin. Experimental results obtained with BSA are expected to be general and applicable to other globular proteins. In this work we aim to study the effect of pH and surfactants at different concentration of BSA solutions and the relevance of these results in protein aggregation. dependence

**Study of Diffusion and Solubility of Hazardous Materials in Polymers using Inverse Gas Chromatography**  
*REU Student: Phoebe Nelson, Department of Chemical Engineering, Pennsylvania State University*  
*Graduate mentor: Ida Balashova*  
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Poly(vinyl) chloride (PVC) meets specifications, such as, plasticity, rigidity, stability, etc… though adding chemicals. Some of these additives may be toxic and are not chemically bound to the polymer. It is possible they will diffuse out of the PVC into their surroundings.

Using Sulfonated Polymers to Dope the Electrode Interface in OPVs
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Organic photovoltaics (OPVs) or polymer solar cells have the potential to drastically reduce the cost of clean, renewable energy because they are much less expensive to produce than silicon-based photovoltaics. OPVs are also lightweight and flexible, allowing them to be used in a wide variety of applications where an inorganic solar cell would be impractical. However, they are not yet efficient enough to be commercially viable on a large scale.

Diffusion and Solubility of Polymer Solvent Systems
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Styrene acrylonitrile copolymer (SAN) is a commonly used polymer. Foamed SAN is created using a blowing agent such as 1,1,1,2-tetrafluoroethane (R-134a). Chloro- and fluoro- substituted hydrocarbons are detrimental to the ozone layer and therefore contribute to global warming. It is useful to understand their interactions with SAN in order to evaluate their rate of release from products.
Ionic liquids (ILs) are nonvolatile salts that exist as liquids below 100 °C. These materials have a variety of diverse properties that include non-flammability, high thermal stability, high ionic conductivity, and wide redox stability. The combination of properties found in ILs has made applications that were
hindered by the volatility of conventional solvents feasible. Energy management is among the fields where ILs have drawn considerable interest. Replacing the volatile, flammable electrolytes found in present day batteries with ILs could viably offer several important advantages, including increased operating ranges and longer battery life. Most importantly though, ILs would provide a significant safety improvement due to its nonflammable and nonvolatile properties, curtailing the risk of internal pressure build-up and thermal runaway. Using ILs in electrochemical systems have their share of drawbacks as well. Most notably these include poor mechanical performance, low Li ion transference, and ineffectiveness in arresting dendrite growth. Tethering ILs to a nanoparticle such as Polyhedral Oligomeric Silsesquioxane (POSS) could be an effective way to create a high-performance electrolyte that does not suffer from the aforementioned limitations. POSS is well suited for this purpose due to qualities arising from its rigid chemical structure, allowing higher mechanical stability and reducing dendrite formation2.

Site-Specific Doping for Organic Photovoltaics

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**PEDOT:PSS** is regularly used as the hole transport layer in organic photovoltaics (OPVs), despite its hydrophilicity, opaqueness, and high acidity. To researchers, it presents problems such as corruption of devices over time and inhibited photon absorption. By examining the performance of alternative modifying layers, the PEDOT:PSS problem may be mitigated and OPV output increased to a profitable level.

Dissipative Particle Dynamics Simulations to Model Calcium Phosphate Nanocomposites

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[http://www.matse.psu.edu/faculty/colina](http://www.matse.psu.edu/faculty/colina)

Calcium – phosphate (CP) based materials offer a nontoxic, biodegradable platform for biomedical devices. However, drug delivery and bioimaging applications are limited by phase changes at physiological pH. Successful delivery vehicles must sustain an amorphous state in order to encapsulate and deliver molecules in vivo. The force on bead i is given by:

\[
\text{conservative force (repulsive) dissipative force (frictional)}
\]
Random Force Dissipative – Random Force Relations Atomistic computer simulations of large systems such as ACP are difficult due to the large quantities of atoms present. Dissipative particle dynamics (DPD) can be used to represent large and complex atomic arrangements.