

physiological function of mucus, and are involved in disease progression.

Bioconjugation of fluorescent nanoparticles with target molecules for human breast cancer

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BACKGROUND AND OBJECTIVES
The encapsulation of molecules in calcium phosphosilicate nanoparticles (CPSNPs) and attaching a target molecule to the surface of the particle serves as an improved vehicle for the delivery of chemotherapeutics and imaging agents to cancer cells or tumors.

RESULTS AND DISCUSSION
I. Absorbance Analysis
The absorbance of Rhodamine WT (Rh-WT) at different concentrations was measured to create a standard curve on a Multiskan plate reader. The standard curve is used to determine the concentration of dye in the particles. The concentration of Rh-WT and the absorbance are directly proportional.

EXPERIMENTAL PROCEDURES
Synthesis of CPSNPs
CPSNPs were synthesized by the sol-gel process using calcium phosphosilicate (CaPSi) as the precursor. The synthesis was carried out in a stirred reactor at 60°C for 24 hours.

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Stability of Nonuniformly Charged Sub-Micron Colloidal Particles

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Background
Nonuniformly charged sub-micron colloidal particles are ubiquitous in nature and are of great interest to researchers in fields such as paints, cosmetics, and drug delivery devices. While classical theories such as the DLVO theory assume charge uniformity on the surface of these particles, these theories often fail to accurately predict repulsive forces for Brownian particles. Furthermore, there are currently limited experimental studies on measuring charge nonuniformity of submicron aggregates. Submicron aggregate stability differs from larger particles since these particles are difficult to settle under gravity, more challenging to view under an optical microscope, and

Results
Customizing Aggregate Length Based on Settling Out Time
The aggregate length of sub-micron colloidal particles can be customized based on their settling out time. The aggregate length increases as the settling out time increases.

Angular Velocity vs. Aggregate Length
The angular velocity of sub-micron colloidal particles decreases as the aggregate length increases. The angular velocity is inversely proportional to the aggregate length.

Conclusions
The aggregate length of sub-micron colloidal particles can be customized based on their settling out time. The aggregate length increases as the settling out time increases. The angular velocity of sub-micron colloidal particles decreases as the aggregate length increases. The angular velocity is inversely proportional to the aggregate length.

Sub-micron colloidal particles are auspicious candidates for technology such as paints, electronics, cosmetics, and drug delivery devices. While classical theories such as the DLVO theory assume charge uniformity on the surface of these particles, these theories often fail to accurately predict repulsive forces for Brownian particles. Furthermore, there are currently limited experimental studies on measuring charge nonuniformity of submicron aggregates. Submicron aggregate stability differs from larger particles since these particles are difficult to settle under gravity, more challenging to view under an optical microscope, and

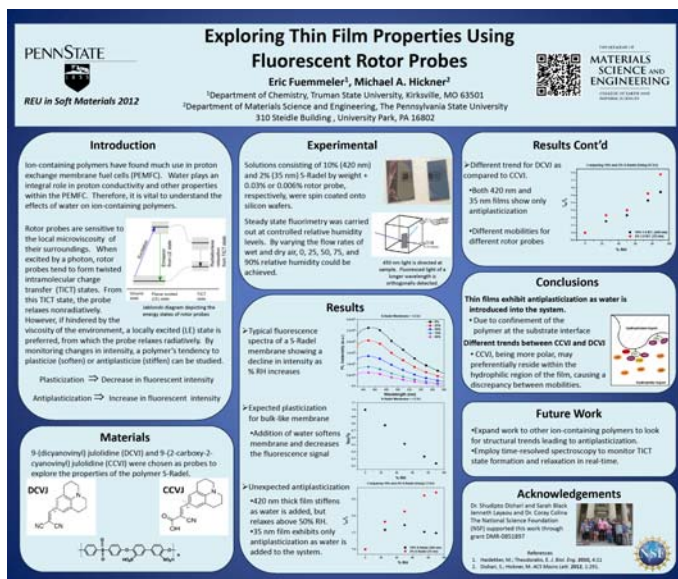
more responsive to shear. In this study, charge nonuniformity of sub-micron colloidal aggregates has been quantified by measuring the angular velocity as a function of aggregate length under rotational electrophoresis. It has been shown that the angular velocity, and thus the charge nonuniformity of the aggregates, decreases with increasing aggregate length.

Exploring Thin Film Properties Using Fluorescent Rotor Probes

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Ion-containing polymers have found much use in proton exchange membrane fuel cells (PEMFC). Water plays an integral role in proton conductivity and other properties within the PEMFC. Therefore, it is vital to understand the effects of water on ion-containing polymers. Rotor probes are sensitive to the local microviscosity of their surroundings. When excited by a photon, rotor probes tend to form twisted intramolecular charge transfer (TICT) states. From this TICT state, the probe relaxes nonradiatively. However, if hindered by the viscosity of the

environment, a locally excited (LE) state is preferred, from which the probe relaxes radiatively. By monitoring changes in intensity, a polymer's tendency to plasticize (soften) or antiplasticize (stiffen) can be studied.

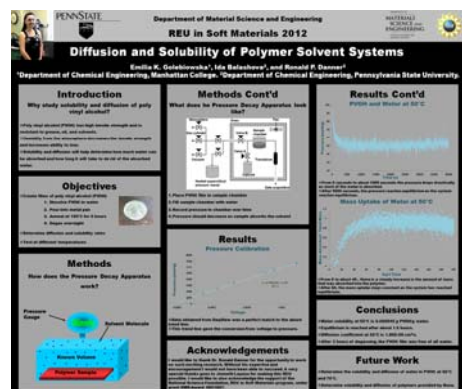
Diffusion and Solubility of Polymer Solvent Systems

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Poly vinyl alcohol (PVOH) has high tensile strength and is resistant to grease, oil, and solvents. Humidity from the atmosphere decreases the tensile strength and increases ability to tear. Solubility and diffusion will help determine how much water can be absorbed and how long it will take to de rid of the absorbed water.

Separating Oil from Tar Sands using Ionic Liquids (IL)

REU Student: Stephanie Santos Díaz, Chemistry Department at University of Puerto Rico, Cayey

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Separating Oil from Tar Sands using Ionic Liquids (IL)
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Experiment #1
Tar Sands
Mixture of clay, sand, water and bitumen.
Recovered bitumen – source of fuels.
Conventional processes of bitumen separation require a great amount of hot water - energy.
IL's are effective to separate bitumen from tar sands; H₂O is used only to wash IL from solids.

Background and Goals
What are Ionic Liquids?
IL: Large organic cations and anions that melt at or below 100°C; have an outstanding chemical and thermal stability; non-flammable at ordinary temperatures.
Used with non-polar solvents to separate bitumen from oil sands.
Separation: at ambient temperature, no use of water in the primary step of separation.
Goals
1. Use the least amount of resources
2. Extend the technology to other problems, for example: environmentally oriented
3. Get a clean separation
4. Economic: cost of separation is approximately \$5 per barrel of bitumen produced.

Experiment #2
Speed of the separation process
Working at industries, speed is essential.
Additives to speed up? IPA?
When compared, the speed rate is similar.
Centrifugation – for better separation
FTIR – to monitor quality of products
Conclusion: The new additive results in a cleaner separation.

Conclusion: Using IL results in an effective separation. Washing it from the residue solids means IL can be 'recycled', which lowers the cost of IL Replacement.

Mixture of clay, sand, water and bitumen. Recovered bitumen – source of fuels. Conventional processes of bitumen separation require a great amount of hot water - energy. IL's are effective to separate bitumen from tar sands; H₂O is used only to wash IL from solids. Using IL results in an effective separation. Washing it from the residue solids means IL can be 'recycled', which lowers the cost of IL Replacement.

Molecular Modeling Of Blood Plasma Factor XII (FXII)

REU student: Julie Soderlind, Department of Materials Science and Engineering, Washington State University

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Molecular Modeling Of Blood Plasma Factor XII (FXII)
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¹ Department of Materials Science and Engineering, Washington State University, The Pennsylvania State University

BACKGROUND
All known cardiovascular biomaterials cause blood to clot (coagulate) leading to dangerous medical complications such as stroke. Biomaterial contact with FXII (Hageman factor), causes an enzyme initiating the cascade. The activation mechanism is unknown but dependent on material surface chemistry. The enzyme splits into different fragments depending on the cleavage site.

OBJECTIVE
The objective of this study was to build a realistic model of the catalytic domain of FXII and use it to determine how the presence or absence of disulfide bridges affects the catalytic domain of the enzyme.

METHODOLOGY
• Atomistic molecular simulations were performed - every atom represented explicitly.
• The Amber 10 software was used with the CHARMM force field.
• The initial conditions for each simulation were experimentally determined protein conformational information.
• Added a constant force to monitor cleavage process.
• Simulated in 3D.
• 100 ns simulation with 1000000 steps.
• 25 trajectories of FXII in any direction between the protein and the "new" wall.
• Used periodic boundary conditions.
• Long equilibration process, multiple parallel settings.
• 1 - Water reduced, Amber force field.
• 2 - Water reduced, Amber force field.
• Large-scale simulation used to slow temperature from 300K to 200K, holding protein fixed at constant temperature for 20 picoseconds.
• Then held entire system at constant temperature (200K) and pressure (1atm).
• A total production run of 2 microseconds, with time step of 2 femtoseconds.

RESULTS
Density, temperature, volume, and root mean square were monitored.
A steady state in 1 ps in respect to protein volume and conformation in water at the conditions stated in this work. One disulfide bond of the catalytic site does not appear to make any significant structural changes during the length of the present simulation.
Snapshots of the simulation with hydrogen aligned show that only the residues 177 and 171 make a structural change when treated. The disulfide bond of the catalytic site does not appear to make any significant structural changes during the length of the present simulation.

CONCLUSIONS
The simulation of the catalytic domain with a disulfide bridge showed stable steady conditions. One that with a broken disulfide bridge. Future work:
• The simulation should be run for longer times to determine true stability.
• Molecular will be useful according to a review.

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[3] Yeh, F., S. H. Yeh, S. H. Yeh, S. H. Yeh, and S. H. Yeh, "The Role of the Substrate of Factor XII in the Activation of Factor XII", *Biochemistry*, 2009, 48(17), 4000.

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REU in Soft Materials

All known cardiovascular biomaterials cause blood to clot (coagulate) leading to dangerous medical complications such as stroke. Biomaterial contact with FXII (Hageman factor), creates an enzyme initiating the cascade. The activation mechanism is unknown but dependent on material surface chemistry. The zymogen splits into different fragments depending on the cleavage site. Fragments created may be neutral, activate other proteins (amidolytic) or cause amplification of the cascade (procoagulant). Understanding how and why these fragments form is

critical in creating a biomaterial with a surface structure that does not cause clotting. It is hypothesized that residues 26 and 42 contain the disulfide bridge that holds the chain together after activation.

Virtual Swelling of Polymers of Intrinsic Microporosity

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Polymers of intrinsic microporosity (PIMs) are a new class of glassy polymers which have a rigid, contorted backbone that allows for inefficient packing and inherently creates free volume (pores < 2 nm). PIMs have potential use in applications such as gas separation and storage.

Integral to understanding the properties of PIMs is understanding the nature of swelling. PIM-1 (below) has been shown to have a high selectivity and diffusivity compared to other polymeric materials, as illustrated (right) by the Robeson plot, but swelling decreases membrane effectiveness

Inclusion Concentration and Precipitate pH Influence the Degree of Amylose Inclusion Complex Formation with Dicarboxylic Fatty Acids

REU student: Michael Vilkhovoy, Department of Chemical Engineering, University of Massachusetts

Graduate mentor: Abhishek Kar,

Faculty advisor: Dr. Darrell Velegol

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Oil from dead-end pores cannot be extracted by pressure driven flows. Extracting plugs from these dead-end pores can be done through ion gradients which can be imposed or self generated. Our research examined the use of imposed salt gradients which are able to generate spontaneous electric fields in these systems.

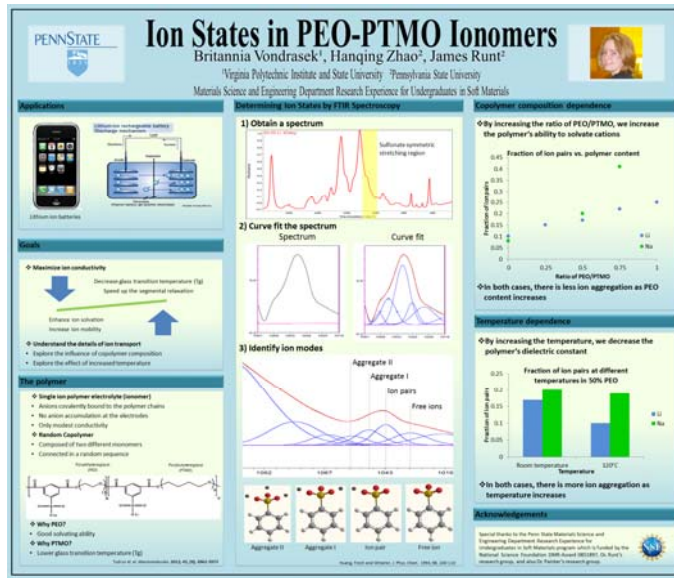
Ion States in PEO-PTMO Ionomers

REU student: Britannia Vondrasek, Virginia Polytechnic Institute and State University

Graduate mentor: Hanqing Zhao

Faculty advisor: Dr. James Runt

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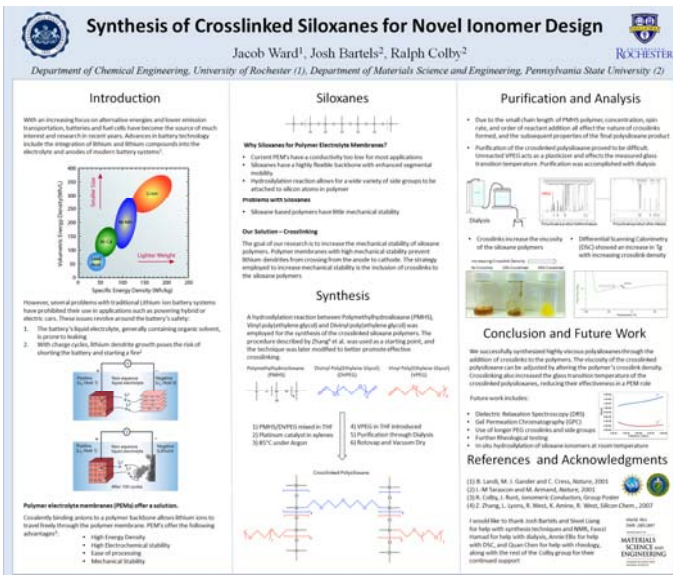
Synthesis of Crosslinked Siloxanes for Novel Ionomer Design

REU student: Jacob Ward, Department of Chemical Engineering, University of Rochester

Graduate mentor: Josh Bartels

Faculty advisor: Dr. Ralph Colby

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With an increasing focus on alternative energies and lower emission transportation, batteries and fuel cells have become the source of much interest and research in recent years. Advances in battery technology include the integration of lithium and lithium compounds into the electrolyte and anodes of modern battery system