REU in Soft Materials at Penn State
2012 Research Projects

Molecular Simulations of Organic Molecules of Intrinsic Microporosity

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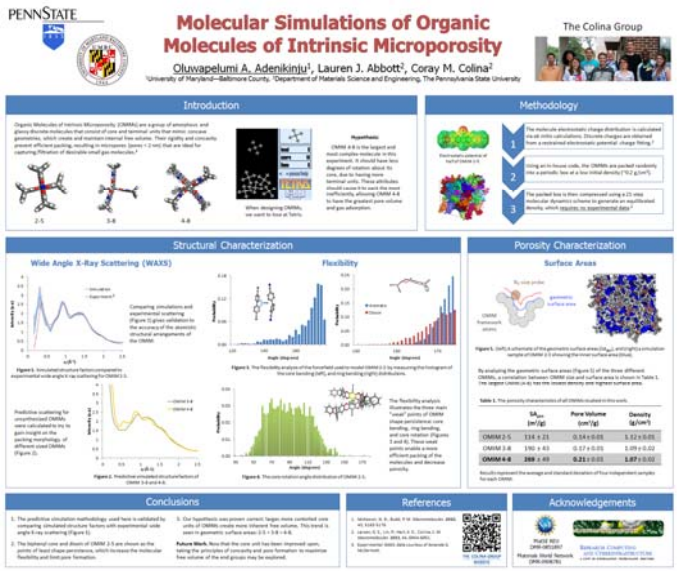

Organic Molecules of Intrinsic Microporosity (OMIMs) are a group of amorphous and glassy discrete molecules that consist of core and terminal units that mimic concave geometries, which create and maintain internal free volume. Their rigidity and concavity prevent efficient packing, resulting in micropores (pores < 2 nm) that are ideal for capturing/filtration of desirable small gas molecules.

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Mucin Aggregation from Molecular Simulations

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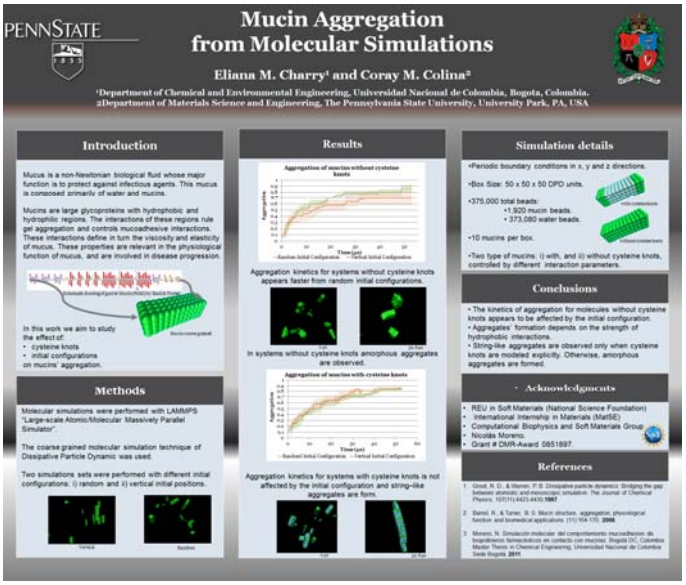

Mucus is a non-Newtonian biological fluid whose major function is to protect against infectious agents. This mucus is composed primarily of water and mucins. Mucins are large glycoproteins with hydrophobic and hydrophilic regions. The interactions of these regions rule gel aggregation and controls mucoadhesive interactions. These interactions define in turn the viscosity and elasticity of mucus. These properties are relevant in the

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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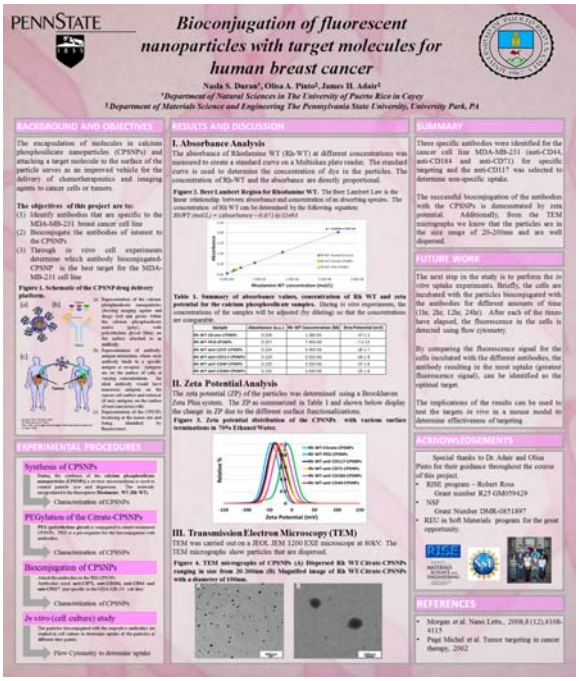

The encapsulation of molecules in calcium phosphosilicate nanoparticles (CPSNPs) and attaching a target molecule to the surface of the particle serves as an improved vehicle for the delivery of chemotherapeutics and imaging agents to cancer cells or tumors.

Stability of Nonuniformly Charged Sub-Micron Colloidal Particles

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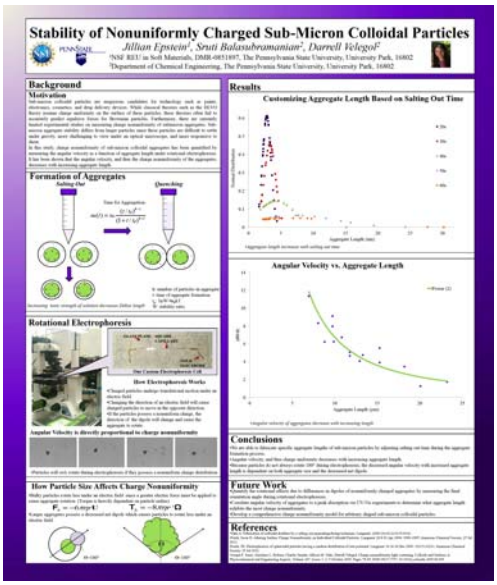

Sub-micron colloidal particles are auspicious candidates for technology such as paints, electronics, cosmetics, and drug delivery devices. While classical theories such as the DLVO theory assume charge uniformity on the surface of these particles, these theories often fail to accurately predict repulsive 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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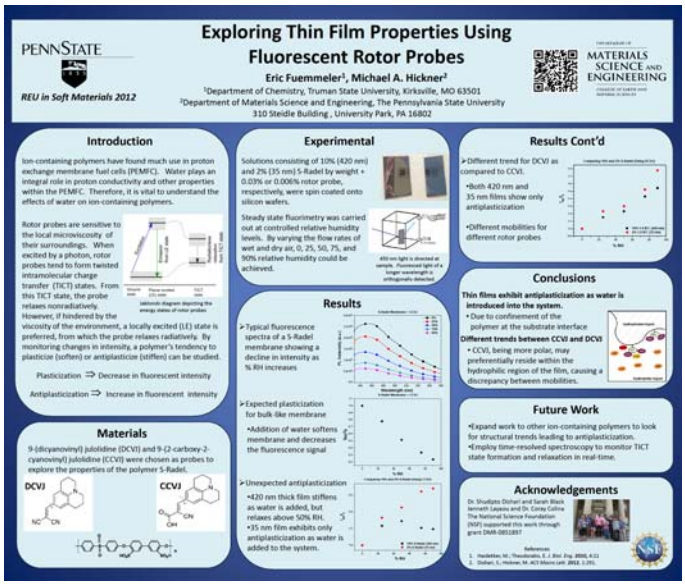

Ion-containing polymers have found much use in proton exchange membrane fuel cells (PEMFC). Water plays an integral role in proton conductivity and other properties within the PEMFC. Therefore, it is vital to understand the effects of water on ion-containing polymers. Rotor probes are sensitive to the local microviscosity of their surroundings. Whenexcited 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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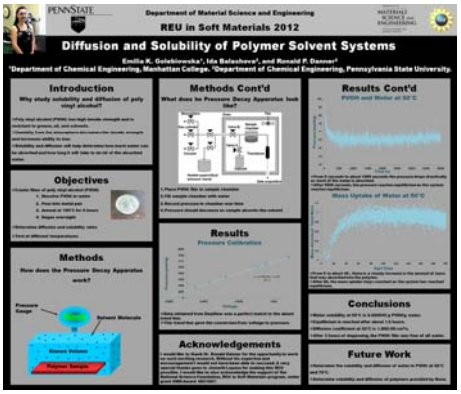

Poly vinyl alcohol (PVOH) has high tensile strength and is resistant to grease, oil, and solvents.Humidity from the atmosphere decreases the tensile strength and increases ability to tear. Solubility and diffusion will help determine how much water can be absorbed and how long it will take to de rid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

Separating Oil from Tar Sands using Ionic Liquids (IL)

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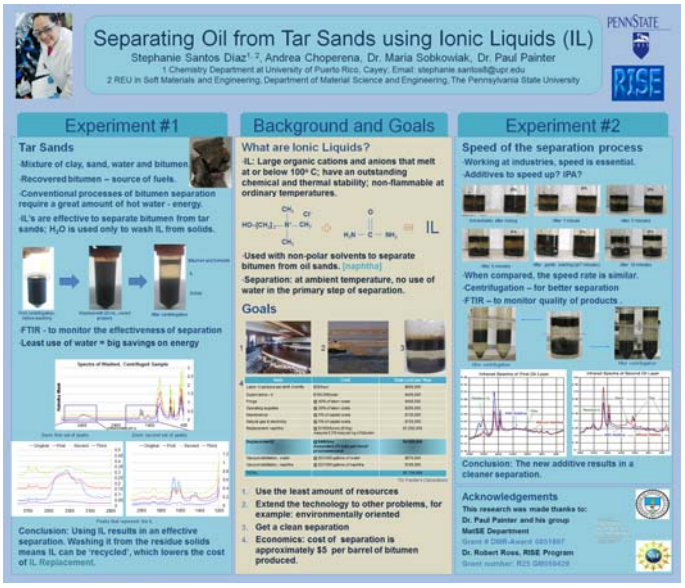

Mixture of clay, sand, water and bitumen. Recovered bitumen – source of fuels. Conventional processes of bitumen separation require a great amount of hot water - energy. IL's are effective to separate bitumen from tar sands; H_2O is used only to wash IL from solids. Using IL results in an effective separation. 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)

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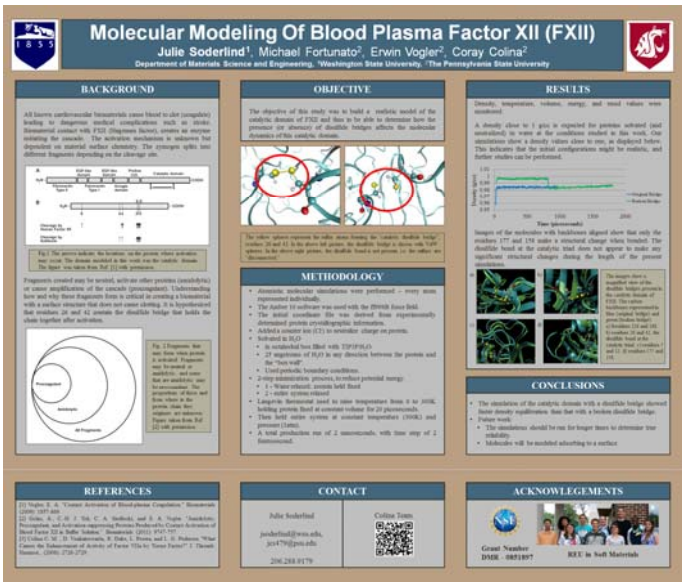

All known cardiovascular biomaterials cause blood to clot (coagulate) leading to dangerous medical complications such as stroke. Biomaterial contact with FXII (Hageman factor), creates an enzyme initiating the cascade. The activation mechanism is unknown but dependent on material surface chemistry. The 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 Microporsity

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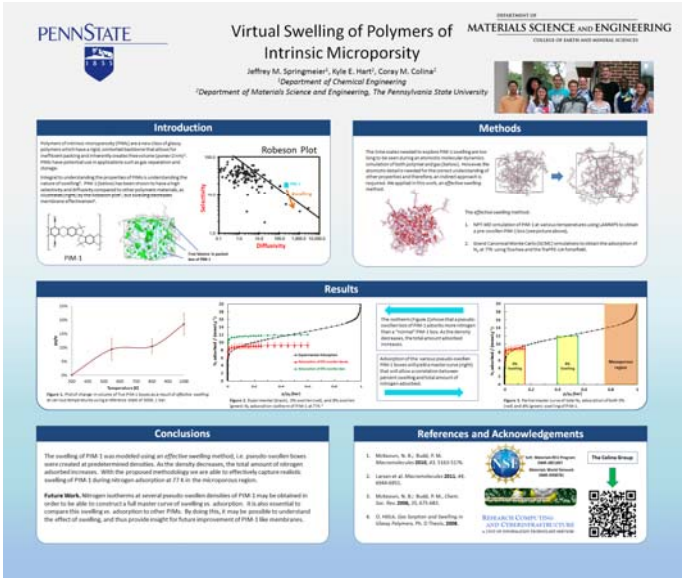

Polymers of intrinsic microporosity (PIMs) are a new class of glassy polymers which have a rigid, contorted backbone that allows for inefficient packing and inherently creates free volume (pores<2 nm). PIMs have potential use in applications such as gas separation and storage.
Integral to understanding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

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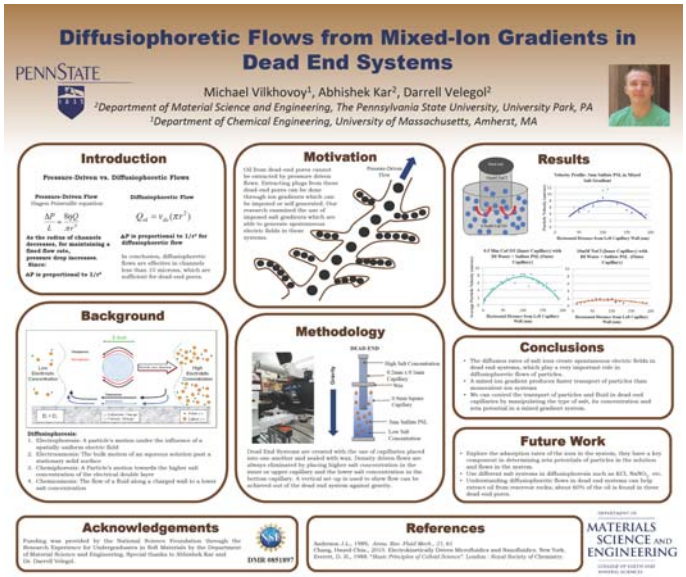

Oil from dead-end pores cannot be extracted by pressure driven flows. Extracting plugs from these dead-end pores can be done through ion gradients which can be imposed or self generated. Our research examined the use of imposed salt gradients which are able to generate spontaneous electric fields in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

Ion States in PEO-PTMO Ionomers

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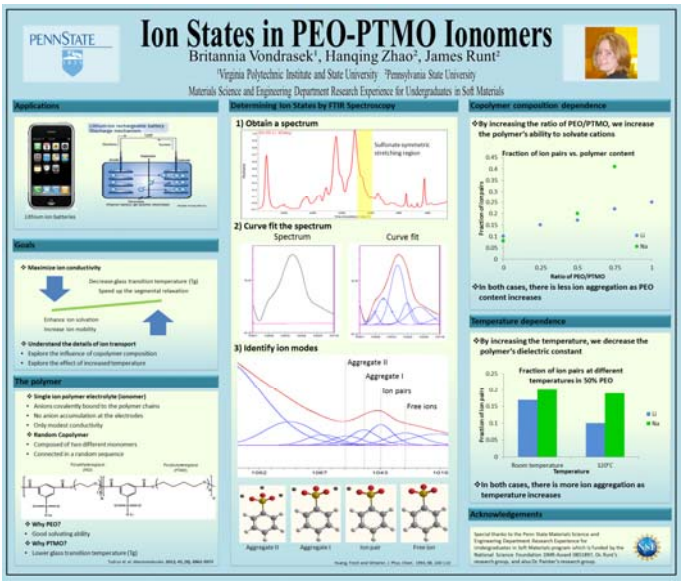

Synthesis of Crosslinked Siloxanes for Novel Ionomer Design

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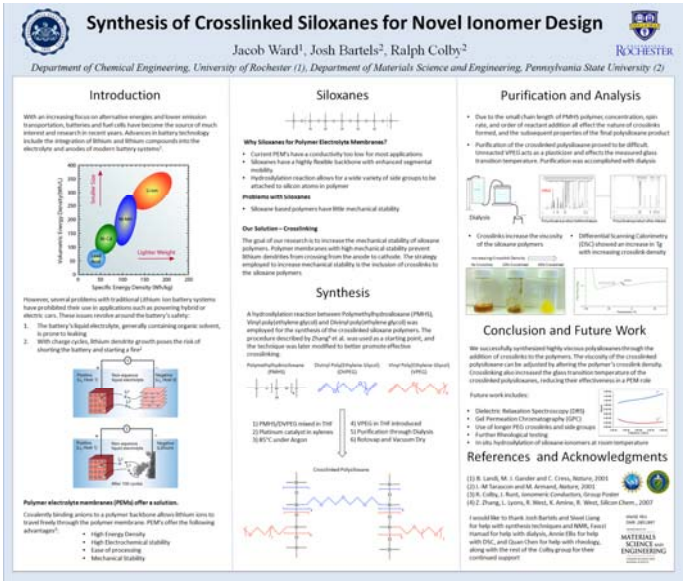

With an increasing focus on alternative energies and lower emission transportation, batteries and fuel cells have become the source of much interest and research in recent years. Advances in battery technology include the integration of lithium and lithium compounds into the electrolyte and anodes of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