



6th Annual Graduate Research Symposium

William G. Lowrie Department of
Chemical & Biomolecular Engineering

The Ohio State University

Abstract Book

2017



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Abstract Book



A.1 The Quaternary State of Polymerized Human Hemoglobin Regulates Oxygenation of Breast Cancer Solid Tumors

Donald A. Belcher and Andre F. Palmer

Hypoxic conditions in the tumor microenvironment induce quiescence in cancer cells, which reduces the effectiveness of cancer therapies. In this study we analyzed how transfusion of polymerized human hemoglobin (PolyhHb) locked in either the tense(T) or relaxed(R) state regulate oxygenation of solid tumors with both computational and animal models. In a modified Krogh tissue cylinder simulation, we explored the effect of varying doses, geometry, and hemodynamics on the oxygen consumption rate and the overall oxygen transfer rate. We found that R-state PolyhHb oxygenated selectively under hypoxic conditions, whereas T-state PolyhHb increases oxygenation at all oxygen tensions. Animal studies with a top-load injection of PolyhHb in mice with the MDA-MB-231 breast cancer cell line resulted in decreased hypoxia and vascular density for both PolyhHbs. Toxicology analysis revealed that the both PolyhHbs cleared primarily through the liver and spleen. These results indicate that R-state PolyhHb is an excellent candidate to decrease tumor hypoxia.



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A.2 Optimizing Biopharmaceutical Manufacturing: Investigating Efficient Protein Expression and Purification Strategies

Merideth Cooper and David Wood

Although affinity tags are commonly used in laboratory settings, tagged proteins cannot be used as therapeutics because of the potential immunogenicity of the tag. In this work, we describe a novel self-cleaving tag technology, based on a highly modified split-intein cleaving element. This purification approach has been combined with cell-free expression systems to reduce the time it takes to produce therapeutic proteins. This method is convenient and effective for the purification of traceless target proteins, and is currently being applied in a BioMOD platform device for on-demand biologics production.



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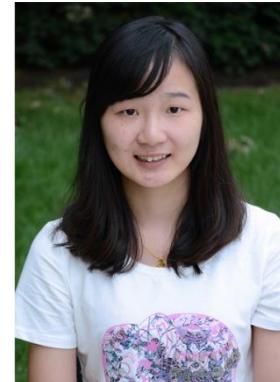
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A.3 Split Intein-based Platform Technology for Recombinant Therapeutic Proteins Purification Process

Yamin Fan and David Wood

The use of recombinant protein for therapeutic applications has increased significantly in the last three decades. While upstream expression level of protein therapeutics being improved remarkably, downstream processing remains the costliest step of biopharmaceutical production and there is considerable demand to reduce the costs involved by using platform technology. Purification tags provide a robust tool in creating a generic platform for purification of a wide range of recombinant proteins with high selectivity and high purity. Over the past decades, inteins have been genetically modified to be implemented in the purification method to overcome the limitation of purification tags. In this work, different designs of signal peptide are used in combination of modified C-terminal cleaving Npu DnaE split intein to facilitate the purification of proteins expressed in mammalian cell systems, which helps to expand the application of such purification platform.



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A.4 Production and analysis of earthworm hemoglobin as a therapeutic oxygen carrier

Richard Hickey and Andre Palmer

Hemoglobin from the earthworm *Lumbricus terrestris* (LtHb) is a gigantic oxygen-carrying protein with appealing qualities for clinical use. Its large size compared to human Hb (3,600 vs 64 kDa) helps avoid many of the complications of extracellular Hb solutions. Here we describe a method for scalable production of LtHb from Canadian nightcrawler worms. Protein is isolated through several stages of micro- and ultrafiltration. Several methods of biophysical characterization provide data about the structure and function of LtHb, including gaseous ligand binding kinetics. The unique oxygen equilibrium curve of LtHb demonstrates its high degree of cooperative binding, a desirable feature for ensuring dynamic delivery of oxygen to tissue. A large, extracellular oxygen carrier such as LtHb has a multitude of potential applications in transfusion medicine and tissue engineering.



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A.5 A Directed Evolution Approach for Engineering Self-Cleaving Intein Affinity Tags Using Yeast Surface Display

Samuel D. Stimple and David Wood

Self-cleaving intein affinity tags have been utilized to purify a wide range of proteins, and allow for recovery of tagless, high-purity protein sample. Although this purification modality appears broadly generalizable, the use of this technology has been largely limited to bacterially-expressed proteins at laboratory scale due to premature cleavage of the intein in mammalian cell cultures. To address this shortcoming, we used a directed evolution approach combined with a yeast surface display-based screen to engineer the ΔI-CM intein, with the objective of isolating mutants suitable for use in mammalian expression hosts. Such inteins would possess tightly controlled cleavage kinetics, exhibiting minimal premature cleavage during expression but retaining the ability to cleave rapidly following a buffer shift. Using our approach, mutants have been identified that i) undergo less premature cleavage during expression in *E. coli* at 37°C, and ii) cleave rapidly after a shift to 20°C and pH 6.0.

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A.6 Exploring network-based strategies to define applicability domain for quantitative structure-activity models

Vinnie Ribeiro and James Rathman

Computational modeling of chemical toxicity is becoming increasingly more important to help guide the drug discovery process by prioritizing and reducing the number of necessary experiments on chemicals to evaluate whether they may be toxic to humans. Quantitative structure-activity relationship models are used to build models based on available experimental data to predict the behavior of a compound for which there are no empirical data. Our objective is to develop a network-based approach using structural information in a dataset to determine groups of compounds that are highly correlated with a given toxicity endpoint. This allows for the creation of an intuitive graphical representation of the data, alongside models with an applicability domain that is more well-defined than the ones that are currently available. This approach will help improve the reliability of predictions obtained from the information present in the dataset.



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B.1 Selective glucose isomerization to fructose using heterogeneous amine catalysts

Nitish Deshpande and N. A. Brunelli

Biomass is an attractive carbon source for a sustainable chemical industry. Selective glucose isomerization to fructose is a bottleneck in upgrading cellulosic biomass to high valued products like high fructose corn syrup and useful intermediates like 5-hydroxymethylfurfural. Lewis acidic Sn-beta zeolite has been extensively researched as a heterogeneous catalyst for this reaction in the past few years. Recent reports demonstrating the ability of homogeneous amines to selectively convert glucose to fructose offer an alternate to Sn-Beta and immobilized enzymes. There is a growing interest in developing means to translate these properties of homogeneous amines to heterogeneous materials. Herein, we report heterogeneous amine catalysts developed using silica-based supports for selective conversion of glucose to fructose. Different catalyst design parameters including the amine length and loading that affect the catalyst performance are evaluated and tuned to get the best catalytic performance.



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B.2 High Temperature Co-electrolysis of Carbon Dioxide and Water to Produce Synthesis Gas

Dhruba J. Deka and Umit S. Ozkan

Carbon capture and sequestration have found immense importance in last few decades. Recent research works are focused on conversion of this captured CO₂ back into hydrocarbon fuels. In this study, a solid oxide electrolysis cell is employed to co-electrolyze CO₂ and water into a mixture of CO and H₂, also known as synthesis gas. The cell is operated at 600-800°C and consists of yttria-stabilized zirconia (YSZ) electrolyte, lanthanum doped strontium titanate cathode and lanthanum doped strontium manganite anode. YSZ conducts oxygen ions at elevated temperatures (>500°C). CO₂ and H₂O get reduced at the cathode to form CO, H₂ and oxide ions. These oxide ions then travel through the YSZ electrolyte and combine to form molecular oxygen at the anode. Syngas so produced can be converted into liquid hydrocarbon fuels by Fischer Tropsch synthesis. If a renewable power source supplies the electricity required for electrolysis, the fuel cycle can become carbon neutral.



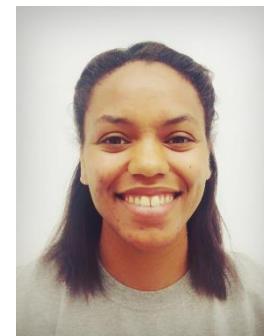
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B.3 Utilizing solvent-effects within heterogeneous catalysts for selective production of 5-hydroxymethylfurfural (HMF)

Mariah R. Whitaker and N. A. Brunelli

Biomass, such as lignocellulose, is an abundant carbon source giving it great potential as a green alternative to fossil resources as a renewable source for production of chemicals and fuels. Current methods break lignocellulose down into its monomeric components, which are converted to useful platform chemicals such as 5-hydroxymethylfurfural (HMF). Previous research has shown that organic solvents stabilize HMF preventing it from being converted to byproducts, increasing HMF selectivity. The current challenge for HMF production is achieving high selectivity in water alone to avoid the difficult separation of HMF from the bulk organic solvent. This study involves implementing organic-like solvent effects within a mesoporous silica catalyst to promote fructose dehydration to HMF selectively in water. We find that the catalytic material design can impact the catalyst performance, resulting in high selectivity. Overall, this work provides a new direction to tune catalytic activity and selectivity.



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B.4 Catalytic Treatment of Water Contaminated with Chlorinated Hydrocarbons

Gokhan Celik and Umit S. Ozkan

Contamination of groundwater by chlorinated compounds such as trichloroethylene (TCE) is an environmental concern due to their high level of toxicity and potential impact on drinking water. Existing remediation techniques for treatment of contaminated water are not efficient or feasible due to low rates of remediation, high energy inputs, and media regeneration/replacement cost. Although hydrodechlorination (HDC) appears to be an efficient way of groundwater remediation, it suffers kinetically due to low concentration of contaminants and catalyst deactivation due to anionic groundwater constituents. The focus of this study is the use of a new class of materials, namely swellable organically-modified silicates (SOMS) as a catalyst scaffold for HDC reactions. When used as catalyst scaffolds, SOMS can have potential to resolve the issues involved in HDC of TCE. In this study, the catalytic activity and poison resistance of Pd-incorporated SOMS have been investigated for HDC of TCE. A wide variety of characterization techniques have been used for a better understanding of the nature of these materials.



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B.5 Regioselective alcohol ring opening of epoxides using Lewis acidic catalysts

Nitish Deshpande and N. A. Brunelli

Epoxides are versatile chemical intermediates that can be conveniently synthesized from alkenes. Various nucleophiles like water, alcohols, amines, and thiols can open the epoxide ring yielding synthetically important di-substituted compounds. Low selectivity and/or stability of different heterogeneous acids and bases that can catalyze this reaction have limited their scope. In this work we have studied silica-based Lewis acidic catalysts with varying pore-sizes and Lewis acid-site strength. We report that these catalysts can selectively open the epoxide ring using alcohols under mild conditions for different systems including epichlorohydrin-methanol. Systematic investigations of the effect of acid site strength, temperature, and pore-confinement of these materials reveal that these factors affect the catalytic activity but not the regioselectivity. In case of terminal mono-functional epoxides, the regioselectivity increases with an increase in nucleophile size. Overall, we present catalytic performance and reusability of different silica-based Lewis acidic catalysts for epoxide ring opening with alcohols.

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B.6 Synthesis and application of nano zeolites to overcome diffusion limitations in Lewis acid catalyzed reactions

Rutuja Joshi and N. A. Brunelli

A major drawback in zeolite catalyzed reactions is the mass transfer limitations in conversion of large molecules which normally are restricted to access the active sites inside the micropores, resulting in reduced catalytic activity. The potential of nano sized zeolitic material to overcome this limitation for Lewis acid catalysis is being investigated in a variety of manners. This project aims to synthesize Lewis acidic nano zeolites (<100 nm) with MFI topology at low temperature under hydroxide conditions. The crystallization process will be monitored for heteroatom substitution into the zeolite framework. The catalyst is characterized using several analysis techniques such as X-ray diffraction, nitrogen physisorption, Dynamic Light Scattering, and Scanning electron microscopy. The novel catalytic material is then used in batch reaction testing for conversion of bulky reactants. The more precise engineering of zeolites with reduced crystal size and comparison of the catalytic performance with bulk material will allow us to find an efficient route to overcome diffusion limitations of bulky reactants.



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B.7 Enhanced Thermal Management of High Power Electronics Using Carbide-Bonded Graphite Films

Paul Garman and L. James Lee

Due to the ever increasing power density of electronics along with the need of many devices to be able to operate at high voltages and currents, it is imperative that these devices be provided proper thermal management to prevent power degradation and eventual failure. Currently, high power device packages make use of direct-bonded copper (DBC) ceramic substrates; however, the thermal conductivities of the ceramics implemented are relatively low. We have developed a process to deposit high quality graphite films directly onto ceramic substrates via a chemical vapor deposition process. By depositing these films onto the exposed ceramic regions of DBC substrates, we show that we can significantly improve the thermal management of high power devices. Using this process, we can extend device lifetime and efficiency as well as decrease power electronic substrate costs.

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B.8 Preferential oxidation of Carbon Monoxide over Swellable Organically Modified Silica (SOMS) supported Cobalt Oxide

Dishari Basu and Umit S. Ozkan

The global interest in eco-friendly processes has increased the demand for proton exchange membrane fuel cells (PEMFCs). PEMFCs require an ultra pure hydrogen (H_2) stream as the feed gas. However, this feed may contain traces of carbon monoxide (CO) and water vapor (H_2O). As little as 10ppm of CO can poison the platinum anode catalyst present in PEMFCs. Thus, this hydrogen feed stream must be purified. The preferential oxidation (PROX) of CO to CO_2 is a simple and low cost method to reduce the CO concentration in the H_2 feed. Among the relatively inexpensive transition metals, cobalt (Co) based catalysts are highly active for this reaction. However, H_2O present in the H_2 feed considerably decreases PROX performance over supported Co catalysts. Therefore, the aim of this project is to synthesize an inexpensive, hydrothermally stable Co based catalyst by supporting it on a novel hydrophobic material known as swellable organically-modified silica (SOMS).



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B.9 Hetero-atom Doping of Carbon-Nitrogen Nano-structures For Applications in Proton Exchange Membrane Fuel Cells

Vance Gustin and Umit S. Ozkan

One of the key barriers to the commercialization of hydrogen fuel cells is the high cost of platinum catalysts used on the cathode. Nitrogen doped carbon nanostructures (CNx) have been shown as a viable alternative to platinum catalysts for the oxygen reduction reaction (ORR) and represent a significant cost reduction. Investigations into heteroatom doping of CNx have shown potential for further increasing its activity.

CNx catalysts were prepared using chemical vapor deposition of nitrogen and carbon over an iron acetate doped magnesium oxide support at high temperature. The catalyst is soaked in sulfuric acid and filtered to remove the metal based support. Hydrochloric acid soaking of CNx is used to adsorb chloride ions. Cyclic voltammetry, X-ray photoelectron spectroscopy, temperature programmed desorption and Fourier transform infrared spectroscopy were used to analyze the effect of the chlorine dopant on surface composition, species distribution and ORR activity.

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B.10 Dopant modified iron based oxygen carriers for chemical looping applications

Mengqing Guo and Liang-shih Fan

Chemical looping is a promising technology in many fields, such as carbon capture, methane to syngas production. Iron based oxygen carriers, as intermediates, are the most crucial part of the success of chemical looping applications. However, iron oxide itself doesn't have good reactivity with many reducing gases. Dopants can promote the reduction reactions by providing active sites and create schottky defects to increase the ionic diffusion of iron oxide based. In this study, 1 % to 5 % of Ni, Co, Cu or La doped iron oxide oxygen carriers are synthesized and characterized by TPR, MS, XRD, XPS and SEM/EDS. Meanwhile, the DFT method was used to understand the reduction reaction. The understanding of methane to syngas mechanism provides a way for dopant method for improving the reactivity and recyclability of oxygen carriers, which is a promising way to build the oxygen carriers for commercialization success of chemical looping processes.



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B.11 Nature of Active Sites in Nitrogen-Doped Carbon Nanostructures for Oxygen Reduction and Oxygen Evolution Reactions

Deeksha Jain and Umit S. Ozkan

Regenerative polymer electrolyte membrane fuel cell technology has a promising future for sustainable power generation where oxygen reduction (ORR) and oxygen evolution (OER) are two important reactions that take place in the fuel cell mode and electrolyzer mode, respectively. State-of-the-art catalysts for these reactions – Pt for ORR and Ir (or Ru) for OER – are expensive and active only for one of the two reactions, thus necessitating the development of cheaper and efficient bifunctional catalysts for regenerative fuel cells. We have reported nitrogen-doped carbon nanostructures (CNx) to be active, selective and stable for ORR in acidic medium. Our current focus is to evaluate the applicability of CNx as bifunctional ORR and OER catalysts using electrocatalytic activity measurements. We further aim to systematically examine the nature of active sites in these materials using phosphate anions as poisoning probes with the help of various characterization techniques like X-ray photoelectron spectroscopy, Transmission IR and Raman spectroscopy.



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B.12 : Hydrodechlorination of Trichloroethylene Using Pd Supported on Swellable Organically Modified Silica (SOMS) in Aqueous Phase

Saurabh Ailawar and Umit S. Ozkan

Contamination of groundwater by trichloroethylene (TCE) is a major environmental issue due to its high toxicity. Degradation of TCE can be effectively achieved by catalytic hydrodechlorination (HDC). The commercially used catalyst for HDC of TCE is Pd supported on Al_2O_3 which suffers from deactivation by the anions present in groundwater. Herein, a new class of material, swellable organically modified silica (SOMS), is studied to investigate its deactivation resistance. Hydrophobicity of SOMS aids in repelling the anions present in water thereby shielding the active Pd particles. Organics expand the matrix of SOMS, thereby making Pd more accessible to the reactants. We present a comparison between the poison-resistance characteristics of Pd/SOMS and Pd/ Al_2O_3 , supported with aqueous phase reaction experiments and techniques such as inductively coupled plasma optical emission spectrometry (ICP-OES), transmission electron microscopy (TEM) and extended x-ray absorption fine structure (EXAFS). Swellability and hydrophobicity of SOMS, gives it potential to serve as a support for catalytic water treatment processes.



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B.13 Chemical Looping Partial Oxidation of Solid Fuels for High Purity Syngas Production

Tien-Lin Hsieh and Liang-shih Fan

The chemical looping partial oxidation (CLPO) processes presented produce high-purity syngas from solid carbonaceous fuels including biomass and coal. Compared to conventional coal and biomass gasification processes, the CLPO processes eliminate the need for molecular oxygen from an air separation unit (ASU), and deliver increased cold gas efficiencies and decreased fuel consumptions. This study utilized the unique co-current moving bed gas-solid reducer reactors for the partial oxidation of solid fuels to syngas with metal oxide oxygen carriers. The co-current moving bed reactor design provided a desirable gas-solid contacting while minimizing gas bypassing and solid back mixing, which resulted in high fuel conversion and close-to-equilibrium gas composition. The performance of CLPO was successfully demonstrated on a bench-scale reactor with high purity syngas production from solid fuels. The thermodynamic models which accurately predicted the product gas compositions will also be discussed.

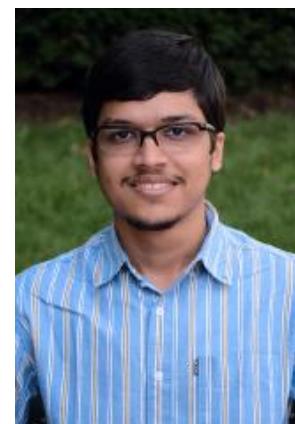
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B.14 Mechanistic Insight for Oxidative Coupling of Methane on Mg₆MnO₈-Based Redox Catalysts in a Chemical Looping System

Deven Baser and Liang-shih Fan

Methane activation has been the topic of interest for many decades for its upgradation to value added chemicals. With the onset of advancements in fracking technology, understanding this C-H bond activation becomes important as it is a key reaction step in the direct synthesis of chemicals from methane. One such method for direct conversion is oxidative coupling of methane (OCM), which provides a single step path towards synthesizing higher hydrocarbons from methane, especially ethylene. A popular way for methane oxidation in OCM is through co-feeding molecular oxygen with methane over a catalyst. Conversely, the chemical looping method utilizes the lattice oxygen in a catalytic oxygen carrier (COC) for methane oxidation. A Mg-Mn-O system was studied under the chemical looping method for understanding the mechanism of OCM with simultaneous oxygen vacancy formation. These effects of vacancy formation were studied using density functional theory calculations.



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C.1 Liquid-Liquid Electrospray: high-throughput nanocomposite synthesis method via Electrohydrodynamic atomization and Flash NanoPrecipitation

Kil ho Lee and Jessica Winter

Despite ongoing efforts of expanding the use of nanomaterials for a variety of applications, the challenge remains in scaling up the standard synthesis methods to produce high quality products. Standard methods are limited to bench level operations, which often encounter mass and energy transfer problems with a lack of control over the precise organization of materials in nanometer scale when attempted to scale up. In response, National Nanotechnology Initiative (NNI) fosters the development of a robust nanomanufacturing platform that could produce high quality nanomaterials in a larger scale that could enlarge the interest of applying nanotechnology further. This study demonstrates a scalable nanocomposite synthesis platform called Liquid-Liquid Electrospray (LLE). LLE is capable of the electrohydrodynamic atomization (EHDA) of a nonconductive fluid inside of a conductive fluid, which enables semi-continuous nanocomposite self-assembly.

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C.2 Homogeneous Nucleation of Carbon Dioxide in a Supersonic Laval Nozzle

Kayane K. Dingilian and Barbara Wyslouzil

Understanding the nucleation of carbon dioxide (CO_2) on a molecular level has significant implications on the future of assessing and countering climate change. In this work, we intend to study the homogeneous nucleation of carbon dioxide in a supersonic Laval nozzle. The nozzles used in this experiment are designed to reach temperatures of $\sim 90\text{-}100\text{ K}$ when argon is the carrier gas. Pressure trace measurements (PTM) along the length of the nozzle provide the data for flow calculations determining nucleation rate, residence time, and other physical properties. Further analysis with Fourier transform infrared spectroscopy (FTIR) and small angle x-ray scattering (SAXS) are used to confirm nucleation and calculate nucleation rate. Experimental results will also be compared to classical nucleation theory and other models to help mend the gaps between predictive methods and reality.



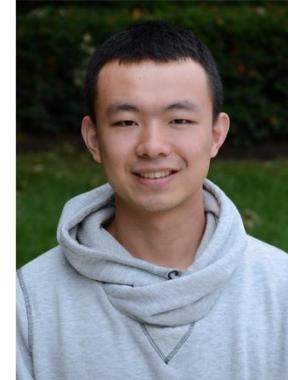
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C.3 Inverse Emulsion Polymerization of Polyvinylamine for CO₂ Capture from Flue Gas

Kai Chen and W. S. Winston Ho

Post-combustion capture of carbon dioxide from the flue gas, generated by coal-fired power plants, is one of the potential methods to reduce carbon emissions. In this work, a composite polymeric membrane was employed to separate CO₂ from N₂. The selective layer of the membrane was made from polyvinylamine (PVAm) blended with an amine-based mobile carrier. The synthesis of PVAm was improved using the method of inverse emulsion polymerization (IEP). As compared to the solution polymerization used previously, PVAm synthesized by IEP had a significantly higher viscosity. Furthermore, the chance of gel formation during the synthesis was reduced. PVAm with a higher viscosity could reduce the penetration of the selective layer into the porous substrate of the composite membrane. It also gave a stronger membrane matrix which allowed a higher percentage of mobile carrier to be incorporated. As a result, the CO₂ permeance of the composite membrane was improved.



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C.4 Structure and Dynamics of Coarse-Grained PEAA Ionomers with and without a Nanoparticle

Janani Sampath and Lisa Hall

Ionomers are polymers containing a small amount of charged groups attached to a non-polar backbone, used in packaging and other applications. We consider a melt of ionomers and their counterions with no solvent, in which the aggregation of ions significantly impacts overall material properties. Prior work established a useful coarse-grained model for acetic acid based ionomers, but considered only fully neutralized materials. To allow clearer mapping to typical experimental systems, we developed a new model that includes unneutralized acid groups with adjusted interaction strengths with each other and with ionic groups. Using this modified model, we simulate a single spherical nanoparticle surrounded by partially neutralized ionomers, considering two different nanoparticle–monomer and nanoparticle–ion interaction strengths. Details of the aggregate morphologies were calculated and compared for systems with and without nanoparticles. We find that aggregates are depleted near the nanoparticle surface, and this increases the segmental dynamics near the surface relative to the bulk..



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C.5 Scale-up of Zeolite-Y/Polyethersulfone Substrate for Composite Membrane Fabrication in CO₂ Separation

Dongzhu Wu and W.S. Winston Ho

A pilot-scale vacuum-assisted deposition setup was developed to continuously deposit zeolite-Y (ZY) nanoparticles on a 14-inch wide nanoporous polyethersulfone (PES) substrate. The deposited substrate was used for composite membrane fabrication for carbon capture from flue gas. The effects of operating parameters, including ZY dispersion concentration, pressure differential, and web speed, on the ZY layer thickness and uniformity were studied. A mathematical model was derived from Darcy's law to correlate the operating parameters to the ZY layer thickness. The model was validated by the parametric study, and the adjustable parameters were determined by fitting the experimental data. After coating an amine-containing polymer selective layer on top of the ZY layer, the composite membrane showed a CO₂ permeance of 800 GPU (1 GPU = 10⁻⁶ cm³ (STP)·cm⁻²·s⁻¹·cmHg⁻¹) with a CO₂/N₂ selectivity over 150 at 57°C, which was superior to the performance of the membrane coated on the bare PES substrate.

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C.6 Novel 2-D graphene- 0-D nanoparticle interfacial composites for potential magnetic functionality

Abhilasha Dehankar and Jessica Winter

Graphene, a 2D monolayer of carbon, exhibits tremendous potential for applications in the semiconductor industry on account of its high electron mobility and strength. However, its lack of magnetism, highly limits its abilities. Prior research failed to produce long range magnetic order in graphene while preserving its electronic properties; however, a recent study succeeded where graphene was placed in contact with a magnetic insulator. Inspired by this work, we are employing superparamagnetic iron oxide nanoparticles (SPIONs) for proximity induced magnetism in graphene with the goal of localized control.

SPIONs are ordered on a silicon dioxide substrate by self assembly using spin, dip or flow coating, followed by graphene transfer to fabricate the composite. The process is analyzed using Atomic and Magnetic Force microscopy and Raman Spectroscopy. Induced magnetism is studied by electron transport Hall effect. This research could result in new approaches to induce magnetism in graphene, permitting possible applications in magnetic storage.



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C.7 Controlling Nanoparticle Size Using Jet-Mixing Synthesis

Pinaki Ranadive and N. A. Brunelli

Nanoparticles are gaining increasing importance in many fields. Their conventional syntheses involve batch processes that have the limitations of low throughput and high variability among batches. The non-uniform thermal and concentration profiles arising from inefficient mixing in a batch reactor lead to a wide particle size distribution (PSD). Mixing is challenging for fast reactions, where it is important for the mixing time to be smaller than the reaction time to generate uniform properties. Flow reactors are attractive alternatives that can improve mass transfer. We illustrate the simple, inexpensive design of a continuous jet-mixing reactor aimed at generating microporous materials of a desired size at high yields. We also examine the mixing dynamics of this reactor to facilitate scale-up. The efficiency of this design is demonstrated by the successful synthesis of zeolitic imidazolate frameworks (ZIFs) of various particle sizes, while future work will involve synthesis of metal and core-shell nanoparticles.

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C.8 PolyDot formulation of Histone deacetylase inhibitor Vornistat, and study of drug encapsulation efficiency and release time

Atefeh Alizadehbirjandi and Jessica Winter

Histone deacetylase inhibitors (HDACIs) are a promising group of agents in cancer treatment. However their poor pharmacokinetics properties have limited the therapeutic efficacy of HDACIs. In this study, we introduce the formulation of Vorinostat (FDA approved HDACI) in micelle templated synthesized nanoparticles (PolyDot system). Using PolyDot system for delivering vorinostat will help with hydrophobicity problem of this HDACI, and enhance drug activity *in vivo*.

PolyDots will be synthesized in a bottom-up synthesis method yielding PLGA/block co-polymer hybrids , consisting of hydrophobic PLGA co-polymers entrapped within self-assembling poly(styrene-b-ethylene oxide) (PS-b-PEO) micelles. Encapsulating Vorinostat by this method provides us with the advantages of two popular drug delivery systems for instance, achieving optimal particle size and high drug encapsulation efficiency.

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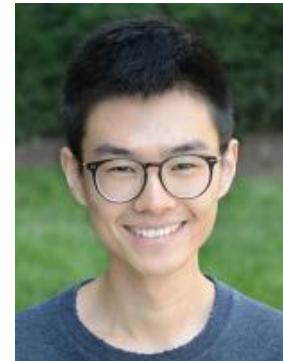




C.9 Techno-Economic Analysis of Polymeric Membrane Systems for Post-Combustion Carbon Capture

Yang Han and W. S. Winston Ho

The increasing consumption of fossil fuels has resulted in immense CO₂ emissions after the Industrial Revolution. Membrane processes have been suggested as an alternative to amine absorption for post-combustion carbon capture. Despite of the tremendous efforts of the membrane researchers, CO₂-selective polymeric membranes typically exhibit a trade-off between CO₂ permeance and CO₂/N₂ selectivity. This presentation will show how to overcome the limitations resulted from this trade-off by novel membrane process designs. In the first membrane process, the combustion air for a power plant boiler is passed to a 2-stage stripping cascade as membrane sweep gas. In the second process, the CO₂-depleted retentate is recycled as an internal sweep for a 2-stage enriching cascade. The techno-economic analysis of the proposed membrane processes shows a capture cost of \$40 – 43/tonne CO₂ with polyamine-containing membrane, which corresponds to a 24% cost reduction compared to amine absorption..



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C.10 Rheology of Shear-banding TTAC Micelles by Constitutive and Rheo-optical Modelling

Xutao Shi and Kurt Koelling

Fracking has been adopted to extract underground natural gas by injecting a fracking fluid into wellbore fractures. However, conventional fluids contain cross-linking additives hazardous to the environment. And the polymer HPG results in post-injection residual that impedes the gas outflow. Therefore, alternative fracking fluids called micellar fluids have been developed, which are environmentally friendly and efficient in gas-yield. However, its rheology is convoluted by micellar structure. In this research, rheology was characterized for different cation/anion ratios. A Giesekus-Diffusion model was implemented and nanostructure was estimated by rheo-optics. Analysis showed that the fluid exhibited shear-banding, represented by stress plateau in rate sweep, and during stress plateau isotropic-nematic phase transition, manifested in birefringence experiments. The current research will result in a better understanding in the rheology and nanostructure of micellar fluids and further its industrial applications such as detergents and central heating.



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C.11 High-Yield Synthesis of ZIF-8 Nanoparticles Using Stoichiometric Reactants in a Jet-Mixing Reactor

Aamena Parulkar and N. A. Brunelli

Zeolitic imidazolate Frameworks (ZIFs) are chemical and thermally stable sub-class of metal organic frameworks. The desirable molecular sieving properties of ZIFs make these materials an interesting candidate for energy-efficient separation techniques, mainly membrane and adsorption techniques. The particle size becomes an important criterion for membrane applications as bigger particles can pose diffusion limitations. The main challenge for greater utilization of ZIFs is the difficulty to synthesize material with uniform particle size and high surface areas at large scales, while achieving high yields. In this work, a solution phase synthesis is demonstrated for ZIF-8 nanoparticles with uniform diameters in the range of 60-80 nm. ZIF-8 is synthesized with 89% yield using stoichiometric precursor concentrations using a jet-mixing reactor. Turbulence created by jets provides homogeneous conditions in the reaction volume resulting in improved yield. The jet-mixing reactor is studied to determine the effect of different synthesis parameters including ligand to metal ratio, base concentration, and mixing intensity. The base concentration has the most effect on the product size, morphology, and yield. The versatility of jet-mixing reactor is shown by synthesizing ZIF-67 with 79% yield. Further, a larger reactor was constructed and tested, demonstrating that the jet-mixing method can be scaled to increase productivity. Overall, this work presents a versatile and scalable route for nanoparticle synthesis.

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Anticipated
Graduation:
December 2018

C.12 Scale-up of CO₂-selective Membranes for H₂S removal in Fuel Cell Applications

Witopo Salim and W. S. Winston Ho

Fabrication of CO₂-selective membrane for H₂S removal was scaled-up by using a roll-to-roll continuous membrane fabrication machine. The scale-up membrane with 14-in wide and > 150-ft length with a selective layer thickness of 15 microns was fabricated by controlling the coating solution, substrate web coating speed, and coating knife gap setting. The scale-up membrane showed the similar performance to the lab-scale membranes. This scale-up membrane was used for the fabrication of prototype spiral-wound membrane modules for a field test with autothermal reformate gas as the feed gas. The modeling and optimization of the membrane process were performed to identify the desirable, recommended test conditions. The field test results achieved > 99% CO₂ removal and 95.7% H₂ recovery, resulting in a retentate hydrogen product stream with H₂S < 10 ppm for the case of wet sweep gas with 40% moisture. These test results agreed well with those predicted by the modeling.



Anticipated
Graduation:
2017

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D.1 Assessing the Domain of Applicability for QSAR Models Predicting Chemical Toxicity

Nicholas Wood and James Rathman

To discover and bring to market a novel drug is a costly endeavor, taking on average \$2.8 billion and 10-15 years. Since the number of potentially synthesizable molecules is seemingly infinite, it is impossible to synthesize and experimentally test every molecule of interest. Therefore, researchers are increasingly turning to computational tools to create models for the prediction of chemical toxicity, a significant cause of drug attrition. These models infer the toxicity of a new molecule from a set of known molecules. Critically, only some molecules can be reliably predicted by the model, a set known as the domain of applicability. The present work develops a method for determining the domain of applicability by extending the notion of chemical similarity to include similarity between a molecule and a set of molecules. A molecule sufficiently similar to the set of molecules used by the model is deemed in the domain.



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Anticipated
Graduation:
May 2018

D.2 Discovering Heuristics for Sustainable Design by Multiobjective Evolutionary Optimization and Machine Learning

Xinyu Liu and Bhavik R. Bakshi

To design a sustainable system, besides quantifying trade-offs between economic and environmental objectives, the knowledge about what makes the solutions optimal is more valuable and can be formulated as design heuristics for guiding future designs of similar systems.



This work integrates the multi-objective evolutionary optimization and a machine learning algorithm, with the main focus on obtaining insights to explain optimality. Both the roles of technologies and nature in engineering design are accounted for explicitly. The methodology has been applied to a case study describing the design of a residential system with multiple technological changes, while accounting for surrounding ecosystems like trees, lawn and a vegetable garden.

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Graduation:
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