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The Ohio State University

Abstract Book

2015

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A.1 High efficiency production of poly (malic-acid) from sugarcane juice by Aureobasidium pullulans

Chi Cheng and Shang-Tian Yang

Poly(L-malic acid) (PMA) is a polymer with great potential in biomedical applications. Its monomer, malic acid (MA), is a widely used food acidulant and has huge commercial value. Industrial sugarcane juice was studied for PMA and MA production by Aureobasidium pullulans ZX-10. Sugarcane juice can be used as a desirable medium for PMA production without any pretreatment, addition of nitrogen or metal salts. Fermentation time from sugarcane juice (110.5 hr) is much shorter compared to pure sucrose (220.5 hr). A PMA production at titer equivalent to 122.0 g/L MA was achieved in fed-batch fermentation with a sugar concentration about 120 g/L in sugarcane juice. Higher productivity was achieved by repeated-batch fermentation by cell-recycle, in the second and third batch, productivity increased 32% (0.665 g/(L·h)) and 85% (0.934 g/(L·h)) compared to the first batch (0.505 g/(L·h)). These results show that sugarcane juice is an efficient renewable feedstock for PMA and MA production, while operating modes such as fed-batch and repeated-batch fermentation can be used to achieve higher titer or productivity.

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A.2 Regulated Oxygenation of Hepatic Hollow Fiber Bioreactors Facilitated by Polymerized Hemoglobins

Donald Belcher, Uddyalok Banerjee, Chris Baehr, and Andre F. Palmer

Tissue engineered constructs are limited by insufficient oxygen transfer. We hypothesize that mixtures of polymerized hemoglobins can both supply and regulate oxygen levels to alleviate constraints in tissue engineering design. This study evaluated the oxygenation potential for mixtures of polymerized hemoglobins (PolyhHb) with dissimilar p50s in a Hepatic hollow fiber (HF) bioreactor. Operation of HF bioreactors are limited by oxygen supply and zonation in the extra-capillary space (ECS). Mixtures of glutaraldehyde polymerized Tense (T) and Relaxed(R) state PolyhHbs were prepared; size, oxygen affinity, and oxygen dissociation kinetics of the resultant mixtures were analyzed. A finite element analysis was performed using the determined biophysical properties of the PolyhHbs to evaluate the dissolved oxygen gradient and oxygen flux across the membrane. We predict that total PolyhHb concentration, T/R state PolyhHb ratios, inlet flow rate, and inlet oxygen tension can be varied to control the ECS Zonation and Oxygen delivery to the cells.

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A.3 Application of Polymerized Hemoglobin to Chronic Wounds to Accelerate Wound Healing

Kristopher Richardson and Andre F. Palmer

Oxygen plays a vital role in the continuous wound healing process, since immune cells at the wound site rely on oxygen for cellular respiration. If the population of immune cells is reduced at the wound site, the wound healing process can be extended for a longer period of time, eliciting the formation of a chronic wound. In the United States, approximately six million people are affected by chronic wounds annually. Hemoglobin (Hb), the protein that transports and delivers oxygen in the body, has been topically applied to chronic wounds to accelerate wound healing. It has been hypothesized that the mechanism that leads to accelerated wound healing is the ability of Hb to facilitate oxygen transport. It has also been hypothesized that Hb may exert therapeutic effects by promoting a pro-healing, anti-inflammatory macrophage phenotype at the wound site, leading to accelerated wound healing in chronic wounds. We hypothesize that by engineering the oxygen affinity of hemoglobin-based oxygen carrier mixtures of tense state and relaxed state polymerized hemoglobin we will be able to identify the exact role each mechanisms plays in healing chronic wounds.

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A.4 Detection of Human Papillomavirus 16 in Squamous Cell Carcinoma of the Head and Neck

Kyoung-Joo Jenny Park and Jeffrey J. Chalmers

Head and neck squamous cell carcinoma (HNSCC) is the most common form of head and neck tumor. Among various causative factors, human papillomavirus (HPV) accounts for 70% of the oropharyngeal cancers that involve tonsils or base of the tongue. Investigating the HPV expression in circulating tumor cells (CTCs) provides specific opportunities because this infectious agent has unique characteristics and a moderately-understood life cycle, which has been linked to different stages of the disease progression. Combined with the negative enrichment and RNA *in situ* hybridization technique, difficulties in analyzing mRNA targets in CTCs are overcome, and visualization of the HPV 16 markers on individual cells is achieved. Experimental results show accuracy, specificity, and reliability of the methodology and further confirm the potential of this study as a tool to provide understanding of the mechanism of the tumorigenesis of HPV-associated HNSCC and the role of CTCs.

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A.5 Development of biosensors to identify new chemicals against dengue fever vectors

Miriam Shakalli-Tang and David Wood

The development of a bacterial biosensor containing a nuclear hormone receptor (NHR) has proven to be an effective alternative to current compound screening strategies that rely on hormone-mimicking properties. NHRs can bind a wide variety of endocrine disruptors in addition to their native hormones. Our allosteric biosensors detect compounds that target NHRs and distinguish between their positive or negative effects on the receptor's activity. When this design is extended from human to insect NHRs, an opportunity arises to screen for potential insecticides against infectious disease vectors. This project seeks to construct a binding sensor in E. coli to favor the identification of those compounds that disrupt the endocrine system of *Aedes aegypti* (Ae), the transmitter of dengue fever. By incorporating the ligand-binding domain of the Ae HR96 into our *E. coli* biosensing plasmid, we are able to detect its response to CITCO, a chemical compound known to be its ligand.

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A.6 Creating an Efficient Biopharmaceutical Factory: Protein Expression and Purification using a Self-Cleaving Split Intein

Merideth Cooper and David Wood

Currently, there is no universal protein purification platform. Moreover, there is no platform that can produce any target protein quickly and inexpensively. The self-cleaving intein tag technology has taken steps to remedy this issue. This technology has been successfully applied in bacterial expression hosts, but premature cleaving in eukaryotic systems is still a problem. If we shift to a split intein, specifically Nostoc punctiforme (*Npu*) DnaE, a large majority of premature cleaving is eliminated, as the intein is inactive until it associates as a full-length intein. Initial work has shown reduction in premature cleaving using a simple protein with no disulfide bonds or glycosylation. The next step is then to show that the split intein system is universally applicable. To do this, the split intein system will be utilized in eukaryotic expression systems, including a cell-free system, to purify more complicated proteins.

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A.7 Detection of exosomes secreted from single cells seeded in a nanofiber-embedded microwell array

Peter Amaya and Jeffrey J. Chalmers

Molecules released by cells (the secretome) in cancer tissue are thought to have a role in intercellular communication and in altering tissue at distant sites making it more amenable to cancer metastasis. We have developed a microdevice capable of analyzing the secretome of single cells isolated from a heterogeneous population. We plan to seed and incubate cell lines in microwells to test the ability of the microdevice to capture exosomes from single cells. Fluorescent antibody labeled captured exosomes are expected to produce a fluorescent spot corresponding to each microwell. We hypothesize that the variance in signal intensity among the fluorescent spots produced by exosomes secreted from viable cells will be greater than the variance in signal intensity from fluorescent spots produced by filling the microwells with a purified exosome solution.

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Anticipated Graduation: Spring 2017

A.8 Targeted Delivery of Therapeutic Gaseous Ligands (CO and NO) for the Treatment of Ischemia Reperfusion Injury

Uddyalok Banerjee and Andre F. Palmer

Hemorrhagic shock is sudden loss of blood volume which induces tissue ischemia, characterized by limited O_2 transport to tissues. Re-establishment of blood flow and restoration of tissue oxygenation is known as reperfusion. Abrupt changes in tissue oxygenation can elicit multiple organ dysfunctions by activating cytotoxic injury processes. These injuries are known as Ischemia Reperfusion Injuries (IRIs).

We hypothesize, HBOCs can be used to deliver potent gases such as CO and NO to ischemic tissues in order to treat IRIs. Ligand loaded HBOCs are expected to supply these beneficial gases to ischemic tissues in order to mitigate IRIs. Additionally, these particles can restore blood volume and shear stress, thereby promoting increased endothelial NO synthesis. After these gases dissociate from the ligand carriers, the carriers are expected to store and transport O_2. The novel therapeutic proposed in this study can be an economical alternative for current IRI treatment strategies.

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Anticipated Graduation: Autumn 2015

B.1 Methane to methanol conversion: Using paired acid sites in microporous materials

Nitish Deshpande and Nicholas A. Brunelli

Methanol is an ideal intermediate for utilizing the abundant methane to produce value added products. Current catalysts are incapable of selectively converting methane to methanol, and the industrial process requires multiple energy intensive steps to achieve this reaction. Creating a catalyst capable of low temperature, highly selective oxidation would be industrially important. In nature, particulate methane mono-oxygenase (pMMO) enzymes catalyze this reaction under ambient conditions by employing a di-copper active-site. Recently, pMMO-inspired Cu-exchanged zeolites have been developed that can produce methanol at low temperatures with high selectivity (~98%). Their inability to give closed catalytic cycles and the low yield (10-15 µmol methanol/g catalyst) obtained because of the low concentration of the paired-Cu active-sites (~5-10%) in these catalysts limits their applicability on an industrial scale. Thus, this project will create novel synthetic methods to create a high density of paired-Cu active-sites through synthesizing uniform paired acid sites in microporous materials.

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B.2 Carbon Monoxide and Hydrogen Sulfide Poisoning on Nitrogen Doped Carbon: a Density Functional Theory Study

John Borror and Aravind R. Asthagiri

Current technology for proton exchange membrane fuel cells relies on platinum as a catalyst for oxygen reduction. One alternative to platinum is nitrogen doped carbon materials (CNx). One of the problems with CNx materials is that the exact catalytic site is not known. We developed a model of these nitrogen doped carbon materials. Then we performed density functional theory calculations to investigate the adsorption of CO and H_2S on nitrogen doped carbon. Experimentally CNx materials are not poisoned by CO and H_2S while platinum and Fe-CNx materials are poisoned. By comparing our model with these experimental results we narrowed down the number of possible catalytic sites for these materials. CNx materials have the potential to reduce the cost associated with PEM fuel cells.

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B.3 Hydrodechlorination of Trichloroethylene over Swellable Organically-modified Silica (SOMS)

Gokhan Celik and Umit S. Ozkan

Groundwater contamination by trichloroethylene (TCE) is an environmental concern due to its toxicity level and its impact on groundwater. Hydrodechlorination of TCE appears to be an efficient and cost effective alternative way of decontaminating groundwater. Although promising catalytic activities have been obtained with the palladium-based state-of-the-art catalysts, deactivation due to reduced sulfur and chlorine species (SO_4^{2-}, HS^-, Cl^-) is still a recurring issue. To overcome this issue, we are planning to use a newly-developed material, swellable organically modified silica (SOMS) as a catalyst support. The deposition of the active metal inside the pores has been facilitated by organometallic precursors used for catalyst synthesis. Hydrophobicity plays an important role to protect the active sites from ionic contaminants. Herein, use of SOMS as a scaffold for Pd-based catalyst is investigated for hydrodechlorination of TCE reaction. Activity measurements performed in liquid and gas phases as well as characterization results will be presented.

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B.4 Designing Microenvironments to Promote Enantioselectivity of Organocatalysts

Mariah Whitaker and Nicholas A. Brunelli

Intriguing small, metal-free organic molecules called organocatalysts are emerging as important highly selective materials. Like enzymes, organocatalysts are designed to utilize acid-base cooperative interactions to catalyze C-C bond forming reactions important for pharmaceutical synthesis. While highly useful, organocatalysts are typically employed at high concentrations, making product purification difficult and costly. We seek to create a heterogeneous version of these powerful homogeneous catalysts. The key challenge is designing an immobilization strategy to ensure the highly enantioselective homogeneous catalysts can achieve high enantioselectivity as heterogeneous catalysts. By immobilizing an analog of the enantioselective Takemoto's catalyst to mesoporous silica, high selectivity can be achieved by a heterogeneous catalyst with uniform active sites. In addition, further design of the microenvironment around the catalyst can allow our catalyst to perform cascade reactions with a single green solvent in a flow reactor, avoiding the need for costly purification of synthetic intermediates.

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B.5 Oxygen Reduction Reaction (ORR) Performance of Nitrogen-containing Carbon Nanostructures (CN_X) and Iron-Nitrogen-Carbon (FeNC) Catalysts in Acidic Media

Kuldeep Mamtani and Umit S. Ozkan

In spite of significant research work towards the development of transition metal containing carbon materials as oxygen reduction reaction (ORR) catalysts for proton exchange membrane (PEM) fuel cells, the nature of their active sites remains debatable. There is evidence that metal is an integral part of an active site whereas other studies show that it is the pyridinic-N coordinated to the edge planes of carbon is the active site. The current study tries to shed light on this debate by studying the effect of acid-washing and sulfur treatment on iron-nitrogen coordinated catalysts supported on carbon (FeNC) and nitrogen doped carbon nanostructures (CN_X). Surface and bulk characterization experiments were also performed to gain valuable insights into these materials. Our results suggest that metal is an essential part of an active site for FeNC catalysts whereas it remains encased within the carbon nanostructure for CN_X ones, hence not participating in ORR.

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B.6 Steam Oxidation Studies of Fe_2O_3-based Oxygen Carriers Using Al_2O_3, $MgAl_2O_4$ and TiO_2 as Support Materials for Chemical Looping Gasification

Ankita Majumder and Liang-Shih Fan

Chemical looping gasification is an efficient, economic and sustainable means for electricity and/or chemicals production with inherent CO_2 sequestration ability. It is based on the high temperature cyclic reduction and oxidation (redox) of metal oxide based oxygen carriers, producing CO_2/syngas, H_2 and heat in three separate reactors. This study investigates the steam oxidation performance of Fe_2O_3 based oxygen carriers using Al_2O_3, $MgAl_2O_4$ and TiO_2 as support materials. Fixed bed steam oxidation of all the three oxygen carriers exhibited steam conversion values >75%, close to the thermodynamic predictions. XRD analyses reveal that different oxides of iron form complexes with TiO_2 and Al_2O_3, while no complexes are seen in the case of $MgAl_2O_4$. $MgAl_2O_4$-supported Fe_2O_3 oxygen carrier is further studied in a magnetic suspension balance with H_2 reduction and steam oxidation for 20 redox cycles, where it exhibited excellent recyclability, with almost no drop in reactivity over time.

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B.7 Multiscale Modeling of Reduction Chemistry on PdO surfaces

Minkyu Kim and Aravind R. Asthagiri

Palladium oxide (PdO) thin film can grow on Pd catalyst surface during oxygen rich conditions. This PdO surface changes the performance of Pd catalyst. To investigate the performance changes, the fundamental understanding of growth, decomposition and reactivity of the PdO surface is necessary. In this work, we study thermal reduction of PdO(101) surface which has been proposed to be important in Pd oxidation catalysis. To do this, the Density Functional Theory calculation (DFT) and the kinetic Monte Carlo (kMC) simulation are used. Through the combination of DFT and kMC simulations, we find autocatalytic behavior and oxygen vacancy chains during the thermal reduction of PdO(101) surface. These results agree qualitatively with the experimental results. Moreover, the results validate our previous claim that autocatalytic behavior stems from the reduced phase which is not formed randomly but forms the oxygen vacancy chain.

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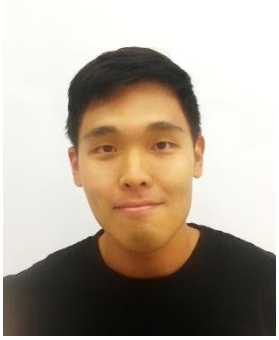

Anticipated Graduation: Spring 2019

B.8 Stoichiometric solution synthesis of ZIF-8 using novel scalable jet-mixing reactor

Aamena Parulkar and Nicholas A. Brunelli

Metal organic frameworks (MOFs) have drawn immense attention in past two decades because of their interesting structure and significant potential for membrane and adsorption applications. Zeolitic imidazolate frameworks (ZIFs), a subclass of MOFs are set of materials with desirable molecular sieving properties for energy-efficient separation techniques. 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. In this work, we demonstrate a stoichiometric solution phase synthesis of ZIF-8 with yield up to 75% using novel jet-mixing reactor. Turbulence created by jets provides homogeneous conditions in the reaction volume resulting in improved yield. The surface area and micropore volume of the synthesized materials confirm the high quality of products. Overall, the work focuses on flow crystallization of ZIF materials using novel jet-mixing reactor.

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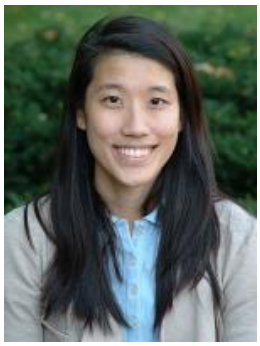
Anticipated Graduation: Spring 2018

B.9 Comparison of Converting Methane to Olefins via Traditional Catalysis and Chemical Looping with Manganese-Based Oxides

Elena Y. Chung, William K. Wang and Liang-Shih Fan

With the global shale gas boom, interest has increased in upgrading methane to olefins. Direct methods of converting methane have been limited by process economics. Since the 1980s, oxidative coupling of methane (OCM) showed promise in producing olefins. Traditional co-feed OCM schemes use gaseous oxidants to catalytically convert methane to ethylene, lowering process efficiencies by requiring energy-intensive air separations. Alternatively, the chemical looping technology presents an opportunity to convert hydrocarbons to flexible products utilizing an oxygen carrier. This study compares the co-feed to the chemical looping approach. Reducible manganese-based oxide catalysts or oxygen carriers are examined in a fixed bed reactor. The results are used in process simulations to model the commercial co-feed system and chemical looping system. Pressure and steam have an effect on ethylene yields. Initial simulations demonstrate that with proper heat integration, the OCM chemical looping process exhibit promise for an alternative direct approach to utilize methane.



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B.10 A DFT Study of CO Poisoning Effects on FeN_XC Oxygen Reduction Reaction Catalysts

Qiang Zhang and Aravind R. Asthagiri

FeN_XC catalysts have been extensively studied for the oxygen reduction reaction (ORR) in fuel cells. However, the nature of active sites is still in debate. We used Density Functional Theory (DFT) to examine CO poisoning effects on possible Fe basal and edge sites. The Fe atom is the sole adsorption site for both O_2 and CO on all sites examined, showing the Fe atom is directly involved in the ORR reaction. O_2 adsorption is affected by N coordination number and pore size while CO shows similar adsorption energy and configuration across all Fe site types examined. Results show only FeN_4C exhibits CO poisoning effect which is consistent with experimental observations that ORR reaction is only partially or weakly poisoned by CO. FeN_2C edge sites exhibit very strong binding towards O_2, suggesting edge sites may not be active towards ORR reaction due to poisoning of OH group.

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B.11 Wash-Coat Development for NO_x Reduction with Methane under Lean-Burn Conditions

Sreshtha S. Majumdar and Umit S. Ozkan

A dual-catalyst after treatment system consisting of a physical mixture of a reduction catalyst (Pd/SZ) and an oxidation catalyst (Co/CeO_2) has been developed for emission control of nitrogen oxides (NO_x), unburned hydrocarbons (CH_x) and carbon monoxide from natural gas-fired lean-burn engine exhausts. This dual-catalyst system utilizes the hydrocarbons, primarily methane, present in the exhaust stream of lean-burn engines for reducing NO_x. Time-on-stream activity tests have demonstrated good hydrothermal stability of this system.
For practical use of the dual-catalyst after treatment system, development of a catalytically active washcoat is essential. As a first step, commonly used binders such as alumina, boehmite and silica, were incorporated into the reduction catalyst. The performance of the modified dual-catalyst bed was tested under simulated engine-exhaust conditions. X-ray diffraction (XRD) and investigation of acid sites with diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) were used to study the effect of addition of binder to Pd/SZ.

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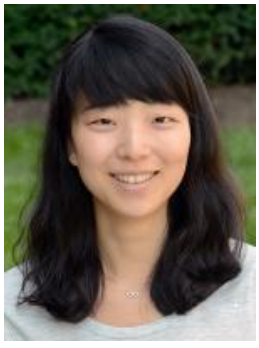
C.1 Enhanced Growth of n-Propanol Nanodroplets in the Free Molecular Regime

Yensil Park, Shinobu Tanimura and Barbara E. Wyslouzil

Investigations by Pathak et al. [*Aerosol Sci. Technol.*, 2013, **14**, 1310-1324] on the growth of nanodroplets in a supersonic nozzle, found that for nonane experimental and theoretical non-isothermal growth rates agreed quantitatively when condensation (q_c) and evaporation coefficient (q_e) were both equal to 1. In contrast, for D_2O nanodroplets, quantitative agreement between experiment and theory during rapid particle growth was only achieved by reducing the evaporation coefficient to ~0.5 while maintaining q_c = 1. One concern with the D_2O experiment was that the droplets were highly supercooled, thereby introducing uncertainty into the analysis since the physical properties for D_2O were extrapolated by up to 50K below the equilibrium melting point. Here we report on similar experiments conducted with *n*-propanol under conditions where droplets are not supercooled. As was observed for D_2O, we find that setting q_c=q_e=1 yields theoretical droplet temperatures up to ~4K lower than those estimated from mass and energy balances, and growth rates that are distinctly below those observed experimentally. Again, better agreement was found by setting q_e=0.6 with qc= 1.0 or, alternatively, setting qc=~1.3 and qe = 1.0. Possible reasons for these differences will be discussed.



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C.2 Freezing of short chain n-alkanes: crystallization to glass formation

Viraj Modak and Barbara E. Wyslouzil

Phase transitions involving straight chain hydrocarbons, or n-alkanes, are encountered in several processes in the industry; for example, polymer processing, supersonic gas separations, or even case of formation of wax deposits, which is an unwanted problem in crude oil transportation. Freezing in n-alkanes is known to initiate at the surface for intermediate chain lengths (15<i<50). We investigate freezing of short chain n-alkane (C8 to C10) nanodroplets, formed in a continuous flow supersonic nozzle. We characterize the flow and the nanoparticles using multiple techniques including static pressure measurements, Infrared spectroscopy and X-ray scattering. Our experiments suggest that these supercooled droplets of short chain n-alkanes also freeze at the surface which is followed by bulk freezing. Furthermore, depending on the inlet conditions to the nozzle we can control whether surface freezing in initiated at the surface or in the bulk as well as control the crystal structure of the frozen particles.

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C.3 The Crystal Structure of Nanosized Ice Particles formed in a Supersonic Nozzle

Andrew Amaya, Viraj Modak, Harshad Pathak, Mike Bogan, Hartawan Laksmono, Claudiu Andrei Stan, Duane Loh, Jonas Sellburg, Raymond Sierra, Sébastien Boutet, Garth Williams, Marc Messerschmidt, Soenke Seifert, Randy Winans, and Barbara Wyslouzil

Supersonic nozzle with cooling rates of about 10^5 K/s are able to probe both vapor-liquid and liquid-solid phase transitions at extreme nucleation rates of ~10^{17} $cm^{-3}s^{-1}$ for vapor-liquid and up to ~10^{22} $cm^{-3}s^{-1}$ for liquid-solid. To examine the structure of ice nanocrystals requires wide angle x-ray scattering experiments with scattering vectors, q, between 1.5 A^{-1} and 3.5 A^{-1}. Experiments at the Free Electron Laser, LCLS, generated 2-D x-ray scattering patterns of ice with concentric rings located at q = 1.72 A^{-1}, 2.79 A^{-1}, and 3.27 A^{-1}. The position and the relative intensities of the peaks suggest that nanometer sized ice crystals created in a supersonic nozzle have a crystal structure that is close to pure cubic ice. To support the FEL experiments, Fourier Transform Infrared Spectroscopy (FTIR) followed the liquid-solid transition for water in more detail, and Small Angle X-ray Scattering (SAXS) determined the size of the ice particles. The SAXS experiments, completed at the Advanced Photon Source (Argonne National Laboratory) on the BESSC 12-ID beamline, found particle sizes of ~10 nm radius. The spectra from FTIR are used to find the fraction of ice, F_{ice}, and together with the particle size to calculate the volume-based nucleation rates, $J_{ice,V}$. The nucleation rates measured here lie between 1.12 x 10^{22} $cm^{-3}s^{-1}$ and 3.17 x 10^{22} $cm^{-3}s^{-1}$. The formation of cubic ice is favored in supersonic nozzle because of the extreme liquid-solid nucleation rates and the small size of the particles.

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C.4 Carbide-Assisted CVD Growth of Graphene Networks on Nonmetal Substrates

Paul Garman and L. James Lee

Formation of graphene films by chemical vapor deposition (CVD) is regarded as one of the most appealing methods for large scale industrial production of graphene. However, the transfer process of moving the graphene film from a metal catalyst to a desired substrate greatly undermines the potential of CVD. Here, we demonstrate a simple and low-cost method for fast and high-coverage graphene growth directly onto various nonmetal substrates with carbide bonding by using atmospheric pressure CVD (APCVD) with methane as the carbon source and poly(dimethyl siloxane) (PDMS) as a silicon free radical source. These graphene networks have superior mechanical properties due to their carbide bonding, as well as high electrical and thermal conductivity, and a low friction coefficient. Potential applications of this technology include but are not limited to fabrication of semiconductor devices as well as thermal management.

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D.1 Fabrication of High Flux Spiral-Wound Membrane Module for Efficient Gas Separation

Witopo Salim and W.S. Winston Ho

Conventional spiral-wound membrane module has a drawback involving the feed gas “bypass” to the feed outlet (retentate) without flowing through the membrane, resulted in lower CO_2 permeance than the flat-sheet membrane. Spiral-wound membrane module comprising face compression “O” rings for effective seal of gases was developed, including the spiral-wound membrane element, Plexiglas FRP (fiber-reinforced plastic) tube, and membrane housing. The membrane modules demonstrated essentially no leakage and the performances were evaluated at 57°C using dry feed gas and sweep gas flow rates of 1000 cc/min at 1.5 and 1 psig, respectively, before their humidification. The transport performance results obtained were CO_2 permeance >700 GPU and CO_2/N_2 selectivity >160, which are twice the CO_2 permeance of the conventional spiral-wound membrane modules. The membrane module is useful for gas separations including post-combustion CO_2 capture in power plants and the removal of CO_2 and H_2S from synthesis gas, H_2-containing mixtures, and CH_4-containing mixtures.

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D.2 Synthesis and Characterization of Polyethersulfone Membrane as Composite Membrane Support Material via Phase Inversion Technology

Dongzhu Wu, Yang Han, Witopo Salim, Varun Vakharia and W.S. Winston Ho

Nanoporous polyethersulfone (PES) membranes were prepared by polyethersulfone/N-methyl-2-pyrrolidone (NMP)/2-methoxyethanol (2-ME) casting solutions. With water as the coagulant, both of the vapor and non-solvent induced phase inversion processes were employed in a successive sequence with varied parameters. A detailed study of the effects of different parameters, including polymer concentration, 2-ME/NMP ratio, relative humidity, water vapor exposure time, and water coagulation bath temperature, was conducted in lab-scale experiments to determine the operation guidelines for pilot-scale continuous machine fabrication. 14-inch wide pilot-scale PES membranes were fabricated with a controlled morphology. Surface morphologies of both lab- and pilot-scale PES membranes were characterized by scanning electron microscopy (SEM). Various effects of the preparation parameters on the lab- and pilot-scale membranes were compared. In addition, Zeolite-Y (ZY) nano-particles were deposited on the pilot-scale PES membrane with a controlled thickness and uniform coverage continuously. PES membranes deposited with ZY particles were applied as the substrate of composite membrane for CO_2 capture from flue gas.

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D.3 Fabrication of Thin-Film Composite Membranes: A Technology Scale-Up

Varun Vakharia and W.S. Winston Ho

Globally, the membrane technology is witnessing a significant growth due to increasing research and development, and market production in chemical, pharmaceutical, biopharmaceutical and life sciences industries. Membranes for gas separation have developed from a laboratory curiosity to a commercial reality due to the low cost and energy efficient alternative for gas separation. Recently, there have been significant breakthroughs in the development of high-flux thin polymer membranes with desirable performance for hydrogen purification and carbon capture applications. This work demonstrates the scale-up fabrication of such membranes via a continuous roll-to-roll membrane fabrication process. Different coating techniques were successfully developed for the fabrication of thin-films (15 µm - 200 nm) on a porous polymer substrate. Composite membranes (14 inches wide and > 500 feet long) were successfully fabricated via the continuous roll-to-roll membrane fabrication process. These membranes demonstrated impressive performances in the industrial field test for the H_2 purification and CO_2-removal applications.

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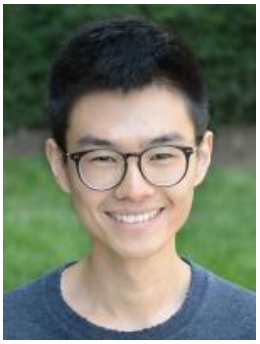
D.4 2-Stage Hybrid Membrane Process for CO_2 Capture from Flue Gas in Power Plants

Yang Han and W.S. Winston Ho



Anticipated Graduation: Spring 2018

Presented herein is a 2-stage membrane separation process for capturing CO_2 from flue gas in a power plant. In the process, the flue gas stream flows to a vacuum membrane stage using a membrane with high CO_2/N_2 selectivity and moderate CO_2 permeance. The retentate gas then flows to an air-sweep membrane stage employing another membrane with high CO_2 permeance but low CO_2/N_2 selectivity. The CO_2 enriched sweep air is passed to the combustor in a power plant. This process shows the lowest cost for CO_2 capture from flue gas in a power plant among various membrane performance properties evaluated.

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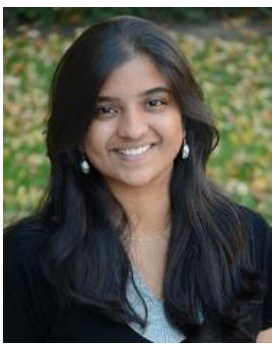
D.5 Emulsion based micellization processes: What is the role played by the surfactant?

Gauri M. Nabar, Barbara E. Wyslouzil and Jessica O. Winter



Anticipated Graduation: Summer 2017

Incorporating hydrophobic nanoparticles into micelles formed from block co-polymers can yield uniform, water-dispersible nanostructures with unique properties. Furthermore, by reducing interactions between the hydrophobic payload and the aqueous environment, the protective matrix can also preserve nanoparticle performance. One popular approach to forming such structures relies on interfacial instability (IS). Here, the amphiphilic block copolymers and the hydrophobic particles are dissolved in a water-immiscible organic solvent such as chloroform, and combined with an aqueous-surfactant mixture to form a emulsion. Micelles incorporating the particles form as the chloroform evaporates. Although surfactant, in our case poly-vinyl alcohol (PVA), is often present at concentrations much higher than that of the amphiphilic polymer, the role the surfactant plays in payload stability is rarely discussed. This talk presents the results of a series of experiments that explores the stability of nanoparticle-loaded micelles as a function surfactant concentration.

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D.6 Molecular Dynamics of Coarse-Grained Ionomers Showing Aggregate Morphology During Deformation

Janani Sampath and Lisa M. Hall

Ionomers are polymers with a small fraction of charged monomers that have a wide range of applications from dental fixtures and packaging to actuators. We consider dense melts of ionomers and counterions with no solvent. An important aspect of their performance is the aggregation of ions, since ionic aggregates act to hold polymer chains together like temporary cross-links. Because of the size scales involved, it is difficult to obtain a complete 3D microscopic picture of polymer aggregation experimentally; typically the thickness of a sample used in transmission electron microscopy is such that multiple overlapping aggregates appear together. How aggregate structure changes under strain and affects mechanical properties is even less clear. We perform molecular dynamics simulations of ionomers of various architectures, and show aggregate morphology and scattering profiles. We apply uniaxial tensile strain and observe the aggregates align, in qualitative agreement with experimental findings. We also obtain stress-strain curves and will discuss effects of degree of neutralization of the ionomers.

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D.7 Molecular Dynamics Simulations of Microphase Separating Tapered Diblock Copolymers

Youngmi Seo, Jonathan R. Brown, and Lisa M. Hall

Tapered AB copolymers consist of pure A and B blocks separated by a middle block whose composition is a linear gradient from pure A to pure B (or from B to A for inverse taper). Prior experiments and theory suggest that one can use taper length as an adjustable parameter to control interfacial and phase behavior, and that tapers potentially make the bicontinuous double gyroid phase more accessible. Using a simple coarse-grained model, we perform molecular dynamics simulations to determine the polymer structure and dynamics as a function of taper length. Generally tapers are seen to increase miscibility and decrease lamellar spacing; the significantly smaller lamellar spacing for inverse tapers is explained in terms of their unique chain conformations. The diffusion and relaxation behavior are closely related to the chain conformations at interfaces. The effect of tapering on penetrant diffusion through one of the microphases will also be discussed.

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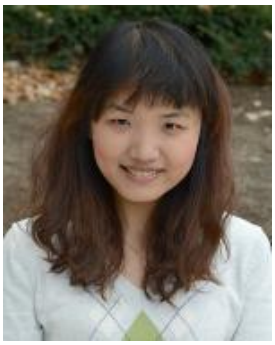
D.8 Water vapor and CO_2 transport through amine-containing facilitated transport membranes

Zi Tong and W.S. Winston Ho

Amine-containing CO_2 facilitated transport membranes have great potential to be applied for hydrogen purification from synthesis gas. In some applications, the humidity of the retentate stream is required as well as the purity of hydrogen. The membranes are highly hydrophilic, and they exhibit not only high CO_2 permeance but also high water vapor permeance. In this work, the transport of water vapor and CO_2 through the membranes composed of an amine-containing selective layer and a microporous polysulfone substrate was investigated. From the experiments conducted, water vapor permeance appeared to be independent of the selective layer thickness, indicating that the substrate is the controlling factor of the mass transfer resistance to water vapor transport. Moreover, water vapor permeance appeared to reduce linearly with increasing the number of the substrate layers. But, CO_2 permeance and CO_2/H_2 selectivity did not change significantly as the number of the substrate layers increased. These results indicated that the CO_2 separation performance is governed by the selective layer as expected.



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D.9 Block Copolymer Micelles with Multiple Morphologies Formed via Electrospray Enabled Interfacial Instability

Matthew Souva, Barbara E. Wyslouzil and Jessica O. Winter

Nanoparticles have tremendous potential in fields ranging from energy to biomedicine. However, much nanoparticle research remains at the bench scale, with little translation to industrial applications. Here, we describe a promising method to synthesize inorganic-polymer composite nanoparticles that combines a scalable electrospray technique with an interfacial instability process to form micellar structures of poly(styrene)-block-poly(ethylene oxide) (PS-b-PEO). This technique has been utilized in batch synthesis to encapsulate and co-localize fluorescent and magnetic nanoparticles in a ~30 nm diameter particle.

To more fully explore the utility of micellar electrospray, we varied operational parameters to increase organic polymer loading and throughput. We were able to demonstrate cone-jet electrospray with increased flow. 15x increases in PS-b-PEO loading led to proportionally increased micelle production. Higher controlled processing temperatures increased micelle production rates versus ambient synthesis. Both empty structures and structures loaded with functional nanoparticles were produced for future applications in payload delivery, imaging, and diagnostics.

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D.10 High Throughput Synthesis of Micellar Nanocomposites via Liquid-Liquid Electrospray

Kil Ho Lee, Barbara E. Wyslouzil and Jessica O. Winter

Self-assembly of amphiphilic block copolymers is a widely studied strategy in generating micelle. Most applications of micelles utilize the structural characteristic with hydrophobic core surrounded by a hydrophilic corona. More specifically, micelles can encapsulate hydrophobic molecules and nanoparticles at the core, enabling efficient drug delivery or bio-imaging. With increasing interest in applying this technology, the production of micelles is usually limited to a batch mode; standard synthesis methods, including sonication, dialysis, and film hydration, are not scalable to produce high quality nanocomposites. In order to achieve higher throughput, our previous work successfully incorporated electrospray with interfacial instability to establish a semi-continuous aerosol based synthesis platform, called Aero-IS. In this work, Liquid-Liquid Electrospray (LLE) is developed to atomize liquid in an insulating bath, achieving high throughput nanocomposites synthesis in the absence of a surfactant for the first time. Based on these recent results, nanoparticle encapsulating nanocomposites were successfully synthesized using LLE.

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D.11 Characterization and Synthesis of site-specific gold nanoparticle: DNA origami conjugates

Abhilasha Dehankar and Jessica O. Winter

Nano machines have wide applications ranging from drug delivery to scalable nanomanufacturing. DNA origami is a promising technology for constructing nano machines because it can generate complex structures with defined components of high strength. In addition, DNA origami structures can be actuated to induce simple manufacturing motions such as transport (i.e., walkers), opening/closing (i.e. scissors, hinges), and sliding/gliding joints (i.e., cylinders). Unfortunately, most DNA structures rely on hybridization/dehybridization kinetics and competitive strand displacement for actuation, which typically result in actuation times of ~ minutes to hours. Here, we describe DNA origami machines integrating nanoparticles with the potential to respond nearly instantaneously. These nanoparticles can stiffen the nanostructure or act as a physical barrier to constrain the motion. Our initial proof-of-concept work demonstrates conjugation of gold nanoparticles at desired locations on dynamic DNA origami nanohinges. We are currently evaluating the potential of nanoparticles to actuate (i.e., open) these structures.

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E.1 Effect of confinement and CO_2 on properties of ethane in nanoporous glass

Sumant Patankar and David Tomasko

High content of higher hydrocarbons such as ethane in certain shales has provided cheap raw materials for petrochemical industries. Confinement behavior of ethane in controlled pore glass (CPG) with nominal pore sizes of 7.5 nm and 35 nm was studied through sorption isotherms and quasi-elastic neutron scattering (QENS) experiments. A magnetic suspension balance was used to measure the adsorption isotherms at 2 temperatures and over a wide range of pressures. The gravimetrically measured isotherms highlight key confinement effects through differences between isotherms for the two pore sizes. Behavior of ethane in the smaller pores was probed further using Quasi-elastic neutron scattering. By measuring the diffusion co-efficient and residence time, we were able to study the effect of pressure and transition to supercritical phase on the dynamics of confined ethane molecules. This study describes physical properties and interactions in the ethane-CPG system under the influence of temperature, pressure and pore-size.

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E.2 From Process to Planet: A Multi-Scale Framework for Designing Techno-Ecological Synergies

Rebecca J. Hanes, Varsha Gopalakrishnan and Bhavik R. Bakshi

Designing sustainable systems requires considering a large, holistic analysis boundary to prevent the shifting of impacts to larger scales while also staying within the carrying capacity of planetary ecosystems. However, conventional process synthesis and design methods lack a holistic approach toward design and also disregard planetary boundaries.
This work introduces the Process to Planet Techno-Ecological Synergy modeling framework that integrates models of industrial, ecological and economic systems at multiple scales. A regional biomass to energy production system is designed using this framework. The design problem includes the farming stage and a biofuel conversion pathway along with supporting ecological systems, a wetland and a forest ecosystem that provides ecosystem services. Technological and ecological design variables are optimized for minimizing ecological impacts and maximizing net present value through the entire system. Results indicate that the proposed approach generates ecologically superior design solutions that are cost effective compared to current solutions.

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E.3 Reducing C and N emissions in US transportation life cycles using Structural Path Analysis

Tapajyoti Ghosh and Bhavik R. Bakshi

Anticipated Graduation: Spring 2019

Determining the hotspots of environmental emissions and material inputs over the life cycle of products is necessary for developing methods to reduce their impacts on the ecosystem. However, life cycle data for individual processes is difficult to obtain, making it imperative to use average economy scale data which is represented as a network of flows in dollars among different sectors. Application of structural path analysis (SPA) to this network enables us to identify sectors corresponding to maximum environmental emissions and resource use. The main objective is to apply SPA to the US economic model for identifying major CO_2 and NO_X emitting sectors for transportation related product demands. Interesting results revealing the pathways for significant C & N emissions were obtained which can guide us to apply process based life cycle assessment only to these key sectors and set up an optimization problem for reducing both of these emissions simultaneously.

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