THE OHIO STATE UNIVERSITY

8th Annual
Graduate Research Symposium

Abstract Book

William G. Lowrie Department of
Chemical and
Biomolecular Engineering

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8th Annual Graduate Research Symposium 2019

Sponsored by The Dow Chemical Co.

Keynote Speaker

Dr. Yatin Gokarn

Global Head of Biologics Drug Product Development & Manufacturing

Yatin joined Sanofi in 2016 and is the Global Head of Biologics Drug Product Development & Manufacturing. Yatin and his teams, based in Framingham, Frankfurt, and Vitry are responsible for the development of clinical, and commercial Drug Products for Sanofi's Biologics portfolio. Drug Development Teams engage early with Biologics Research to enable lead candidate selection, develop drug delivery technical, and then combine formulation & process development, and device integration activities to develop safe, stable, and commercially competitive dosage forms. Yatin also has responsibility for the clinical injectables manufacturing, a network of clinical GMP manufacturing plants.

Prior to joining Sanofi, Yatin led Biologics Drug Product and Device Development at Gilead Sciences, Inc. with prior tenures at Genentech, Amgen, and Pfizer. Yatin has direct experience with successful licensures of multiple biologics and the development of multiple biologics modalities - cytokines, PEG-proteins, Fc-fusion proteins, ADCs, bispecifics, and conventional mAbs in a variety of product formats including liquid and lyo vials, prefilled syringes, cartridges, and pens/auto-injectors.

Yatin is a biophysical chemist (PhD, MS – University of New Hampshire, UNH) and chemical engineering (MS – UNH, BS – Institute of Chemical Technology, Mumbai) by academic training. He serves on the Editorial Advisory Board of the Journal of Pharmaceutical Sciences.

Event Schedule

Time	Event	Venue
8:00 - 8:30 am	Breakfast/Registration	Pfahl Hall 202, the Blackwell Inn
8:30 – 9:00 am	Opening Remarks	Pfahl Hall 202, The Blackwell Inn
9:00 - 9:45 am	Keynote Address	Pfahl Hall 202, The Blackwell Inn
9:45 - 11:00 am	Oral Session 1	Pfahl Hall 202, The Blackwell Inn
11:00 - 11:10 am	Break	Pfahl Hall 202, The Blackwell Inn
11:10 - 12:30 pm	Oral Session 2	Pfahl Hall 202, The Blackwell Inn
12:30 - 2:00 pm	Lunch and Networking	Ballroom ABC, The Blackwell Inn
2:00 - 4:00 pm	Poster session	Ballroom ABC, The Blackwell Inn
4:15 - 4:30 pm	Closing Remarks and Award session	Ballroom ABC, The Blackwell Inn
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10:15-10:30 am	**Jet-mixing Microreactor for Metal and Metal-oxide Nanomaterial Synthesis and Scale-up Considerations** Pinaki Ranadive	7
10:30-10:45 am	**Surface Area Determination of Porous Materials** Archit Datar	8
10:45-11:00 am	**Swellable Organically Modified Silica: A Novel Support for Pd Catalyzed Aqueous Phase Hydrodechlorination of Trichloroethylene** Saurabh Ailawar	9

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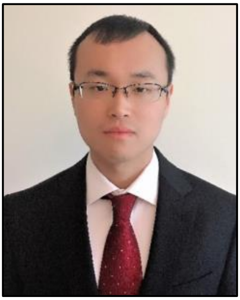
12:00-12:15 pm	**Impact of Microporosity on the Catalytic Activity of Tertiary Amines Functionalized on Silica** Ashwin Kane	13

Process Analysis of an Iron-Based Chemical Looping System for Biogas to Hydrogen Conversion



Presenter: Fanhe Kong
Advisor(s): Dr. Liang-Shih Fan
Email: kong.255@osu.edu
Year of graduation: 2020

Abstract:

Hydrogen (H_2) is a clean fuel and crucial industrial material, but the most commonly used feedstock for H_2 production, natural gas, is not renewable. Biogas can be used as a renewable feedstock for H_2 production to reduce fossil fuel consumption and carbon dioxide (CO_2) emissions. However, the thermal efficiency of the biogas-to-H_2 process is usually significantly lower than natural gas-based processes due to the large energy consumption associated with CO_2 separation. In this research, an iron-based chemical looping technology is investigated as an efficient pathway to convert biogas into H_2 which bypasses CO_2 separation. Sensitivity analysis shows that when the feedstock is changed from pure methane (CH_4) to biogas with 50% CO_2 impurity, the thermal efficiency of the chemical looping system only decreases by 0.4%. Compared to conventional steam methane reforming, the chemical looping process can use ~10% less biogas to produce the same amount of H_2.

Keywords: Biogas, Chemical looping, Hydrogen

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Electrostatic Potential Optimized Molecular Models (ESP-MMs) for Molecular Simulations: CO, CO_2, COS, H_2S, N_2, N_2O, and SO_2

Presenter: Eun Hyun Cho
Advisor(s): Dr. Li-Chiang Lin
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Year of graduation: 2021

Abstract:

Our society is facing critical energy and environment issues; a viable solution is to develop nanoporous materials. However, the large database of nanoporous materials has made the discovery of optimum materials considerably challenging. As a solution, classical molecular simulations play a complementary role in facilitating the materials search. For its reliability, accurate molecular models are of great importance. Therefore, we present a collection of accurate molecular models, including carbon monoxide (CO), carbon dioxide (CO_2), carbonyl sulfide (COS), hydrogen sulfide (H_2S), nitrogen (N_2), nitrous oxide (N_2O), and sulfur dioxide (SO_2). These models are optimized to reproduce the electrostatic potential (ESP) surrounding the molecule and experimental vapor liquid equilibrium. Our calculations verified that a variety of adsorption properties in nanoporous materials can be well predicted with our developed models. We denote this new set of models as electrostatic potential optimized molecular models (ESP-MMs).

Keywords: Molecular models for Molecular simulation

Jet-mixing Microreactor for Metal and Metal-oxide Nanomaterial Synthesis and Scale-up Considerations

Presenter: Pinaki Ranadive
Advisor(s): Dr. Nicholas Brunelli
Email: ranadive.3@osu.edu
Year of graduation: 2020

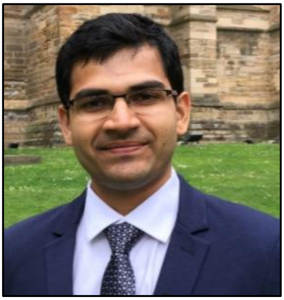
Abstract:

The nanomaterial market is expected to double in three years, requiring technologies that can produce kilogram and larger material quantities while maintaining lab-scale quality. In the lab, nanomaterials are primarily produced via batch processes that are not scalable, since the intense mixing and careful heat transfer control required to produce quality material become inefficient at large volumes. This causes batch-to-batch variability and a wide particle size distribution (PSD). Microreactors that are operated with intense mixing can overcome these challenges. We have developed a simple, inexpensive continuous jet-mixing (JM) reactor for nanoparticle (NP) syntheses. The reactor is successfully tested for Ag NP synthesis. We find that JM results in a narrower PSD, higher shelf life, and 25% lower capping agent requirement compared to batch. The JM system is also adapted for inert synthesis of Cu NPs and Pd@TiO_2 core-shell NPs. To facilitate scale-up, fundamental studies will be done to characterize mixing.

Keywords: Jet-mixing, Microreactor, Nanomaterials, Scale-up

Surface Area Determination of Porous Materials

Presenter: Archit Datar
Advisor(s): Dr. Li-Chiang Lin
Email: datar.10@osu.edu
Year of graduation: 2020



Abstract:

Porous materials have been shown to be promising for use in several environmental applications such as storage of natural gas in natural gas-powered vehicles, capturing water from air, etc. Some of their most important performance parameters for these applications are dependent on their accessible surface area. Thus, the determination of the accessible surface area is an important step in the screening of materials for an application. Traditionally, the BET method has been used for this purpose. However, it has been found that, in some cases, the BET surface area might not be a good representation of the actual accessible surface area. In this study, we discuss the limitations of the BET method and propose ways to supplement it, in order to provide a more accurate surface area prediction.

Keywords: Porous materials, BET theory, Surface area

Swellable Organically Modified Silica: A Novel Support for Pd Catalyzed Aqueous Phase Hydrodechlorination of Trichloroethylene

Presenter: Saurabh Ailawar
Advisor(s): Dr. Umit Ozkan
Email: ailawar.1@osu.edu
Year of graduation: Summer 2020

Abstract:

Swellable organically modified silica (SOMS) is a hybrid organic-inorganic material belonging to the class of bridged polysilsesquioxanes. It has high affinity to organic solvents and is highly hydrophobic. In presence of organic solvents, it undergoes swelling, resulting in increased pore size and surface area. This study investigates the role of SOMS as a catalytic support for degradation of organic pollutants in aqueous media. Hydrodechlorination of trichloroethylene is chosen as the model reaction to study 1%Pd/SOMS. Significant effects of ethanol as the swelling agent on the reaction kinetics and mechanism are discussed. Deactivation resistance of these catalysts in presence of chloride and sulfide species is also investigated. Commercially available Pd/Al2O3 catalyst is used for comparison. Characterization techniques such as, near ambient pressure X-ray photoelectron spectroscopy (NAP-XPS), transmission electron microscopy (TEM), X-ray absorption spectroscopy (XAS), Fourier transform infrared spectroscopy (FTIR), nitrogen physisorption, are used to study the aspects mentioned above.

Keywords: Catalyst, Silica, Hydrogenation, Pd, Hydrophobic

Production of Syngas with Controllable H_2/CO Ratio by High Temperature Co-electrolysis of CO_2 and H_2O

Presenter: Dhruba Jyoti Deka
Advisor(s): Dr. Umit Ozkan
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Year of graduation: Spring 2020

Abstract:

A solid oxide electrolysis cell (SOEC) is a promising renewable technology for CO_2 upgradation. In this device, CO_2 and H_2O are co-electrolyzed at the cathode to produce CO and H_2 (synthesis gas), whereas pure oxygen is obtained as a byproduct at the anode. The primary challenge behind the success of such electrolysis cells is the design of the cathode catalyst. In the current study, a lanthanum strontium ferrite-based perovskite oxide was developed as an SOEC cathode material. The performance of the cathode was found to be enhanced by Fe-site doping with Ni or Co. It was observed that H_2/CO ratio in the product syngas increased with an increase in Ni amount in the cathode material, whereas this ratio decreased with an increase in Co amount in the catalyst. Thus, high energy efficiency and an ability to control the syngas composition makes SOEC a promising route for CO_2 conversion.

Keywords: CO_2 conversion, Synthesis gas, Perovskite oxide

Direct Decomposition of NO_x Using Specialized Metal Oxides in a Novel Chemical Looping Reactor System

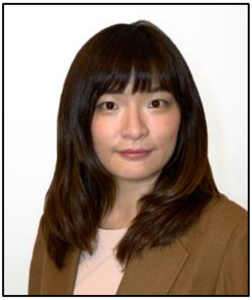
Presenter: Deven Baser
Advisor(s): Dr. Liang-Shih Fan
Email: baser.3@osu.edu
Year of graduation: Summer 2020

Abstract:

NO_x is a potent pollutant that is produced via the flame combustion of fossil fuels. Several strategies for mitigating NO_x emissions employ a reducing agent that selectively reacts with NO_x over a catalyst. Alternatively, NO_x removal can be achieved by direct NO_x decomposition as it is thermodynamically unstable as compared to its decomposition products. This eliminates the use of a reducing agent and incentivizes the direct decomposition process; however, this reaction has a high activation energy barrier, thus imposing kinetic limitations. This study introduces a unique chemical looping reaction system that counters the drawbacks of the direct catalytic NO_x decomposition system using a specialized oxygen uncoupling metal oxide. Here, the metal oxide does not get consumed in the overall chemical looping system, therefore mimicking the direct decomposition reaction with a key difference that it produces N_2 and O_2 products in two separate streams. Findings on the parametric studies on these metal oxides lay the groundwork for this novel NO_x abatement process and will facilitate the advancement of this technology.

Keywords: Chemical looping, Reaction mechanism studies

Synthesis of Sterically Hindered Poly(N-methyl-N-vinylamine) Membrane for CO_2 Capture from Flue Gas



Presenter: Ting Yu Chen
Advisor(s): Dr. Winston Ho
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Year of graduation: 2021

Abstract:

Membrane separation is a potential and advantageous method to capture CO_2 in the flue gas emitted from coal power plants. In the post-combustion capture, both high CO_2 permeance and high CO_2/N_2 selectivity are the requirements to use the membrane process. To achieve high membrane performance, CO_2-amine reversible reaction was utilized in our membrane to facilitate CO_2 transport. High-molecular-weight amine-containing polymer and aminoacid salt were used to synthesis the CO_2 selective membrane. In this work, amine-containing polymer, poly(N-vinylamine) was modified into poly(N-methyl-N-vinylamine) by stepwise reductive amination. Hexafluoro-2-propanol and paraformaldehyde were found to be the effective solvent and the methylating agent for the reaction. Compared to unmodified poly(N-vinylamine), poly(N-methyl-N-vinylamine) demonstrated a higher loading capacity of CO_2 while maintained a sufficient viscosity for membrane coating. As a result, the performance of the composite polymeric membrane was improved by sterically hindered poly(N-methyl-N-vinylamine).

Keywords: Polymer, Membrane, CO_2 capture

Impact of Microporosity on the Catalytic Activity of Tertiary Amines Functionalized on Silica

Presenter: Ashwin Kane
Advisor(s): Dr. Nicholas Brunelli
Email: kane.314@osu.edu
Year of graduation: 2021

Abstract:

Micro-mesoporous materials such as SBA-15 have tunable pore architecture and are used as supports for catalytic applications. Despite widespread use, catalysts functionalized on such materials never reach the activity of their homogeneous counterparts. The key limitation is poor understanding of catalyst-surface interactions. In the present work, we demonstrate that secondary microporosity has substantial impact on the activity of tertiary amine catalysts functionalized on SBA-15. This is shown by reducing the micropore volume in SBA-15 using an updated synthesis procedure. Different surface densities of tertiary amine catalysts are then obtained on conventional SBA-15 and low micropore SBA-15 using the "grafting to" functionalization approach. The catalytic activity of the materials is then tested for the Knoevenagel condensation. Interestingly, the low micropore catalysts consistently give higher activity than their conventional counterparts for all amine densities. Overall, the present work provides fundamental understanding pertaining to effect of micropores on activity of SBA-15 functionalized catalysts

Keywords: Heterogeneous catalysis, Micropores, Mesopores, Knoevenagel condensation, Tertiary amines

Poster Session

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Poster Session

A.1 Magnetophoresis and Spectral Characterization of Deoxyhemoglobin by Conversion with Oxyrase and Sodium Lactate

Presenter: Mitchell Weigand
Advisor(s): Dr. Jeffrey Chalmers
Email: weigand.49@osu.edu
Year of graduation: 2022

Abstract:

A new method for hemoglobin deoxygenation and re-oxygenation is described using EC Oxyrase. This method has several advantages over established methods, such as avoiding side reactions that produce methemoglobin, eliminating the need of a sparging gas and airtight sample as well as easily re-oxygenatation by washing and adding to a normal buffer with dissolved oxygen. Using spectrophotometry, we compare spectra of deoxyHb and metHb with several preparation methods and show the purity of the deoxygenated hemoglobin using oxyrase and its first order reaction kinetics on lysed hemoglobin. Additionally, we demonstrate paramagentism of deoxygenated, intracellular hemoglobin using cell tracking velocimetry and report the effects of hypertonic cell damage on 8-11% of all cells measured in CTV.

Keywords: Oxyrase, Magnetophoresis, Hemoglobin, Paramagnetism

A.2 Synthesis of Polymerized Human Hemoglobin as a Red Blood Cell Substitute

Presenter: Clayton Cuddington
Advisor(s): Dr. Andre Palmer
Email: cuddington.2@osu.edu
Year of graduation: 2022

Abstract:

Transfusion medicine faces compounding problems such as the scarcity of fresh whole blood, concerns with type-matching donor blood to patient blood, and short ex vivo storage lifetime. Polymerized Hb (PolyHb) is one of the most scalable and economical hemoglobin (Hb) based oxygen carriers (HBOCs) currently in development. PolyHb's optimized molecular size will provide a red blood cell (RBC) substitute capable of transporting oxygen while minimizing side-effects such as vasoconstriction, hypertension and oxidative tissue injury. In this study, we synthesized tense quaternary state (T-state) PolyHb using a glutaraldehyde crosslinking agent and analyzed the material's biophysical properties. T-state PolyHb was shown to have a significantly higher molecular weight compared to unmodified Hb, and was purified to remove toxic cell-free Hb and small Hb polymers. This material should facilitate oxygen delivery to hypoxic tissues after transfusion while minimizing potential toxicity and alleviating complications previously observed in early generations of HBOCs.

Keywords: HBOC, PolyHb, RBC substitute, Resuscitation

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A.3 Quantification of The Distribution of Hemoglobin Content in Normal Human Blood Using Cell Tracking Velocimetry

Presenter: James Kim
Advisor(s): Dr. Jeffrey Chalmers
Email: kim.6152@osu.edu
Year of graduation: May 2020

Abstract:

The current clinical method of the detection of low-iron-deficiency-anemia focuses on measuring the amount of hemoglobin in blood. Recent development of particle tracking algorithm and understanding of the relationship between hemoglobin and magnetism has enabled the quantitative measurement of hemoglobin content in RBC based on magnetophoretic mobility. To further explore this relationship, human blood samples has been analyzed by the CTV system, and the calculated hemoglobin concentration data was compared to the values measured from clinical methodology. The results show consistent match between these two methods, and a closer look at the data suggests that the distribution of hemoglobin concentration can provide addition information, indicating that the fraction of RBCs that are below the anemic threshold varies not only from donor to donor, but also in the same donor from week to week. We suggest our cell tracking velocimetry system can reveal more information regarding this matter.

Keywords: RBCs, Magnetism, Particle-tracking, Hemoglobin

A.4 Polyethylene Glycol-conjugated Earthworm Hemoglobin as a Novel Red Blood Cell Substitute

Presenter: Chintan Savla
Advisor(s): Dr. Andre Palmer
Email: savla.11@osu.edu
Year of graduation: 2023

Abstract:

The margin between blood collection and transfusion has seen a consistent annual reduction in the United States and a deficit of 4 million units has been projected by the year 2030. This implies the need for red blood cell (RBC) substitutes. Previous generation HBOCs exhibited Hb extravasation and scavenging of the endothelial vasodilator nitric oxide (NO), eliciting vasoconstriction and hypertension upon transfusion. Lumbricus terrestris (earthworm) possesses an acellular megahemoglobin, or erythrocruorin (LtEc), that may be used as an HBOC. LtEc's large diameter (~30 nm) prevents extravasation of the protein into the tissue to prevent NO scavenging. While LtEc has a short circulatory half-life, conjugation of LtEc with polyethylene glycol (PEG) can lengthen this time in circulation. We have demonstrated successful purification of LtEc from Lumbricus terrestris and PEGylation of this protein. The PEGylated and unmodified species have been compared via size exclusion chromatography (SEC), dynamic light scattering (DLS), O_2 affinity, and cooperativity coefficient (n). PEG-LtEc represents a promising and cost-effective HBOC to reduce the supply strain on trauma treatment centers.

Keywords: Hemoglobin, RBC, Blood substitute, HBOC, Earthworm

A.5 Hemoglobin Nanoparticles as an Oxygen Carrying Resuscitation Fluid

Presenter: Richard Hickey
Advisor(s): Dr. Andre Palmer
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Year of graduation: 2021

Abstract:

Blood transfusion is the gold standard for resuscitation after severe blood loss, restoring much needed capacity for oxygen transport to tissue. However, it is not available in many situations where it is most needed, such as on most ambulances and during remote military deployment. Many attempts have been made to design an intravenous fluid capable of restoring oxygen transport during shock, but few have found clinical success. The present work deviates from classical design in hemoglobin based oxygen carriers (HBOCs) and investigates a new avenue for HBOC development, building on recent advances in biological nanoparticles. Two varieties of hemoglobin nanoparticles are described and evaluated in vitro for biophysical properties and oxygen carrying capacity. They are pathogen-free, type-less, shelf stable transfusion products that appear suitable for use when blood is not available.

Keywords: Medicine, Nanoparticles, Hemoglobin

A.6 DNA Origami Tubes with Reconfigurable Cross-sections

Presenter: Anjelica Kucinic
Advisor(s): Dr. Carlos Castro
Email: kucinic.4@osu.edu
Year of graduation: 2023

Abstract:

Structural DNA nanotechnology, especially the self-assembly process known as DNA origami, enables precise designs with programmed structure, dynamic, and mechanical properties. Advances in dynamic DNA origami include 3D devices with designed 1D motion, such as hinges or sliders, and more complex 2D or 3D motion with actuation capabilities. Recent efforts have sought to extend the function of dynamic DNA origami to material scales through hierarchical assemblies, integrating individual structures into arrays or lattices in a controlled manner. However, to date these assemblies only exhibit simple motion. Reproducing the complex motion of individual devices in larger assemblies remains a challenge. To address this challenge, we developed a reconfigurable 6-component DNA origami mechanism (DOM) that can be reconfigured into multiple shapes and assembled into linear arrays with different cross-sections. Our goal is to demonstrate the reconfiguration of DNA tubes into a variety of stiff cross-sections exhibiting a wide range of mechanical properties.

Keywords: DNA origami, Nanotechnology, Biodesign

A.7 DNA-caged Polymer Nanocomposites for Erasable Fluorescence Imaging

Presenter: Elizabeth Jergens
Advisor(s): Dr. Jessica Winter
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Year of graduation: 2022

Abstract:

The well-known base pairing rules that DNA follows allows for the development of complex two- and three-dimensional structures. These DNA structures can be used in a wide variety of applications including nanoscale engineering and drug delivery. DNA cages, which are designed to form networks on different surfaces, were originally designed by Kurokawa et al. for use as an artificial cytoskeleton inside lipid bilayers. The system proposed here uses the DNA nanostructures to form a cage structure on the surface of polymer micelles and nanoparticles. These cages feature a single-stranded DNA (ssDNA) targeting strand that can reversibly attach to ssDNA via strand displacement reactions. Strand displacement reactions are based on the highest number of complimentary base pairs. Thus, when an ssDNA with greater complement was added, the labeling strand was removed, erasing the signal. These reactions allow for gentle labeling of biological samples without damage, allowing for better labeling of complex samples.

Keywords: Nanomaterials, Imaging, DNA, Nanobiotechnology

A.8 Bench-Scale Production of Glutaraldehyde Polymerized Bovine Hemoglobin as a Red Blood Cell Substitute

Presenter: Xiangming Gu
Advisor(s): Dr. Andre Palmer
Email: gu.606@osu.edu
Year of graduation: 2022

Abstract:

Research in the field of hemoglobin-based oxygen carriers (HBOCs) as red blood cell (RBC) substitutes has been persistently overshadowed by safety issues, such as vasoconstriction, systemic hypertension, and oxidative tissue injury, which are primarily explained by the extravasation of low molecular weight (MW) HBOCs into the tissue space. Currently, there are no FDA certified RBC substitutes for clinical applications in the United States. Hence, the safety issues that have persisted in the development of HBOCs prevents HBOCs from being useful to the warfighter. Previously, our lab investigated the relationship between the MW and vasoactivity of low O_2-affinity, tense-state, glutaraldehyde polymerized bovine hemoglobin (T-PolybHb). We observed that high MW T-PolybHb showed reduced vasoactivity in a top-load model. Hence, our data suggests that the negative vasoactive side effects that have stymied HBOC development can be eliminated by increasing the PolybHb MW. To further optimize this material, we have synthesized a library of high MW T-PolybHb and high O2-affinity, relaxed-state PolybHb (R-PolybHb) of varying sizes and have characterized their biophysical properties.

Keywords: HBOCs, blood substitues, transfusion medicine

B.1 Reducing the Effect of Micropores in SBA-15: Impacts of Mesopore size and Amine-Silanol Interactions

Presenter: Jee-Yee Chen
Advisor(s): Dr. Nicholas Brunelli
Email: chen.8363@osu.edu
Year of graduation: 2023

Abstract:

Mesoporous silica, SBA-15, has attracted attention because of its highly thermally stability and large surface area. Based on our group's previous discovery, eliminating the secondary micropores in SBA-15 can increase both the materials catalytic sites activity and catalytic performance. However, these results brought several further insights, including: (1) previous observations is are based on the incorrect hypothesis which that all the catalytic sites have an equal contribution, and (2) current low micropore materials how to increase the remained have inactive sites in low-micropore SBA-15. Through this study, the pore size effect will be re-examined for low micropore materials, analyzing how the rate constant changes when accurately quantifying the number of catalytic sites under more equal-contribute catalytic site material, low-micropore SBA-15, for eliminating the inactive micropores effect. Secondly, the catalytic activity will be increased by reducing the strong acid-base effect during amine-silanol grafting process, and the amine-silanol interaction will also be further investigated.

Keywords: Pore size effect, Acid-base reaction, Catalyst

B.2 Impact of Microporosity on the Catalytic Activity of Tertiary Amines Functionalized on Silica

Presenter: Ashwin Kane
Advisor(s): Dr. Nicholas Brunelli
Email: kane.314@osu.edu
Year of graduation: 2021

Abstract:

Micro-mesoporous materials such as SBA-15 have tunable pore architecture and are used as supports for catalytic applications. Despite widespread use, catalysts functionalized on such materials never reach the activity of their homogeneous counterparts. The key limitation is poor understanding of catalyst-surface interactions. In the present work, we demonstrate that secondary microporosity has substantial impact on the activity of tertiary amine catalysts functionalized on SBA-15. This is shown by reducing the micropore volume in SBA-15 using an updated synthesis procedure. Different surface densities of tertiary amine catalysts are then obtained on conventional SBA-15 and low micropore SBA-15 using the "grafting to" functionalization approach. The catalytic activity of the materials is then tested for the Knoevenagel condensation. Interestingly, the low micropore catalysts consistently give higher activity than their conventional counterparts for all amine densities. Overall, the present work provides fundamental understanding pertaining to effect of micropores on activity of SBA-15 functionalized catalysts

Keywords: Heterogeneous catalysis, Micropores, Mesopores, Knoevenagel condensation, Tertiary amines

B.3 Synthesis and Catalytic Testing of Tin MFI Zeolite Using Different Tin Precursors

Presenter: Medha Kasula
Advisor(s): Dr. Nicholas Brunelli
Email: kasula.1@osu.edu
Year of graduation: Summer 2020

Abstract:

Zeolites are 3D microporous structures which have been used for catalysis. MFI and beta are the most common zeolites that have been investigated over time for catalysis. MFI zeolite due to its shape selectivity is a very good choice for many commercial processes like cracking and biomass conversion. But due to diffusion limitations there is an observed decrease in catalytic activity of these zeolites. Incorporation of tin in the MFI structure is shown to increase the catalytic activity and selectivity of the Zeolite. Tin(IV) chloride has been traditionally used as the precursor for the Sn incorporation into the MFI. The main aim of this research is to study the effects of tin incorporation using different Sn precursors on the Sn-MFI properties. Properties like crystallization time, morphology and the catalytic activities of the Sn-MFI are studied for different sources of tin like Tin acetate and Tin tertiary butoxide. These properties are compared to that of Sn-MFI synthesized from Tin (IV) chloride for further studies. The study further examines the behavior of the nano Sn-MFI when compared to the conventional Sn-MFI behavior along with different Sn precursors.

Keywords: Nanozeolites, Crystallization time, Conversion

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B.4 Exploring Strategies to Improve Yields of Oxidative Coupling of Methane in a Chemical Looping System

Presenter: Deven Baser
Advisor(s): Dr. Liang-Shih Fan
Email: baser.3@osu.edu
Year of graduation: Summer 2020

Abstract:

Direct conversion of methane to value added products such as hydrocarbons has been a grand challenge for many decades. Although there are several technologies for this, oxidative coupling of methane (OCM) is a promising pathway which is the focus of this study. Under chemical looping mode, methane is oxidized by a catalytic oxygen carrier (COC) instead of molecular oxygen as done in the traditional co-feed OCM, to produce higher hydrocarbons efficiently as the desired product. The objective of this study is to intuitively develop COCs which can achieve high yields in OCM by modifying the base COC. This study focuses on using density functional theory calculations to screen for different metal oxide dopants which are potential candidates that can increase the OCM hydrocarbon yield. The computational results are combined with fixed bed tests of the COCs, which provide the gas-composition data as the reduction proceeds. Results from this study provides key insights into the development of such COCs for the chemical looping application.

Keywords: Methane to Value Added Products, Reaction Mechanism

B.5 Indirect Partial Oxidation of Methane using a Counter-Current Moving Bed Chemical Looping Configuration for Syngas Production

Presenter: Anuj Joshi
Advisor(s): Dr. Liang-Shih Fan
Email: joshi.325@osu.edu
Year of graduation: 2023

Abstract:

Syngas is a key intermediate in producing several commodity chemicals. This coupled with an increase in natural gas availability due to fracking technology has hiked interest in syngas production from methane. In recent years, chemical looping route has gained popularity compared to the conventional technologies such as partial oxidation, autothermal reforming and steam methane reforming. In this study, a novel chemical looping configuration is proposed to the traditional two reactor co-current moving bed chemical looping system. This novel configuration consists of three reactors, a fuel reactor, a syngas generating reactor (SGR) and a regenerator with the fuel reactor and a syngas generating reactor operating in counter current mode with respect to gas-solid flow. The new system called "Indirect Chemical Looping System (IDCL)" increases the syngas yield by favorable thermodynamic equilibrium conditions in SGR. Thermodynamic simulations are performed in Aspen Plus software for analyzing and comparing IDCL under isothermal and auto-thermal conditions.

Keywords: Chemical Looping, Partial Oxidation, Syngas

B.6 Synthesis of Lewis Acidic Nano Zeolite Beta with Increased Hydrophobicity and Chiral Characteristics

Presenter: Alexander Spanos
Advisor(s): Dr. Nicholas Brunelli
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Year of graduation: 2022

Abstract:

Heterogeneous catalytic materials consisting of silica frameworks are important materials for the production of fine chemicals such as pharmaceuticals. One roadblock in the use of zeolite catalysts is caused by diffusion limitations when using large substrates, which can greatly hinder their catalytic activity. This work will focus on tuning the material properties of tin substituted zeolite beta to overcome diffusion limitations through the use of nano zeolites, which because of their smaller size, allow for an increased mobility of reactants. Furthermore, the hydrophobicity of the material will be modified post-synthetically with fluoride. This treatment reduces the amount of silanol (SiOH) defects in the material, thereby improving the catalytic activity and the reusability of the material. Lastly, this work will investigate methods into tuning the enantioselectivity of zeolite beta, which contains natural chiral properties.

Keywords: Zeolite beta, Catalysis, Nanoparticles

B.7 Density Functional Theory Studies of the Role of Defects on $CuFeO_2$ Photocathode Performance

Presenter: Dongjoon Kim
Advisor(s): Dr. Aravind Asthagiri
Email: kim.7270@osu.edu
Year of graduation: 2022

Abstract:

Photoelectrochemical conversion of CO_2 has the potential to produce chemicals and fuels using renewable energy. However, catalysts that are electron efficient, show high selectivity towards desired products and remain stable have proven to be a challenge. $CuFeO_2$, delafossite, is a promising photocathodic semiconductor with a small band gap (1.5 eV). The properties of delafossite, including CO_2 reduction efficiency and selectivity, can be modified through the introduction of defects such as interstitial oxygen and Cu vacancies. We have applied density functional theory (DFT) to understand spectroscopic measurements of the dynamics of electron and hole transfer processes in $CuFeO_2$. Photocurrent improvements can be associated with increasing Cu vacancies, while the inverse occurs with the introduction of O interstitial defects. DFT calculations show that these changes are associated with shifts in the Cu 3d and O 2p states which can promote electron-hole separation and leads to increased photocurrent efficiency.

Keywords: Delafossite, Photocathode, DFT, Defect, CO_2

B.8 Chlorine Poisoning of Nitrogen-Coordinated-Iron-Carbon (FeNC) and Nitrogen-Doped Graphene (CNx) Catalysts in Oxygen Reduction Reaction (ORR)

Presenter: Jonathan Hightower
Advisor(s): Dr. Aravind Asthagiri
Email: hightower.51@osu.edu
Year of graduation: 2022

Abstract:

The adoption of electrochemical energy conversion technologies such as proton exchange membrane (PEM) and alkaline exchange membrane (AEM) fuel cells heavily relies on the choice of catalyst used to increase the activity of the oxygen reduction reaction (ORR). Materials that enhance the ORR have also found industrial usefulness as an oxygen depolarized cathode (ODC) that consumes oxygen to aid in electrochemical chlorine production. Nitrogen-Coordinated-Iron-Carbon (FeNC) and Nitrogen-Doped Graphene (CNx) catalysts offer promising ORR activity and greater cost effectiveness than traditional platinum catalysts. However, FeNC catalysts have been shown experimentally to be poisoned by chlorine, while CNx is tolerant to chlorine poisoning. Density Functional Theory (DFT) calculations show that chlorine adsorbs more strongly than O2 and OOH and blocks the ORR reaction while chlorine binding is weaker on CNx. Experimental data is also generated separately through X-ray photoelectron spectroscopy (XPS) and temperature programmed desorption (TPD) to corroborate computational conclusions.

Keywords: Graphene, Chlorine, Electrochemical, ORR, DFT

B.9 The Potential Utilization of $SrMoO_4$ Anodes for Electrochemical Oxidative Dehydrogenation of Propane

Presenter: Jaesung Kim
Advisor(s): Dr. Umit Ozkan
Email: kim.7261@osu.edu
Year of graduation: 2023

Abstract:

Oxidative dehydrogenation (ODH) of propane is a promising alternate method of propylene production. The steam cracking process has primarily proceeded for propylene production, but it is one of the most energy-intensive processes since high temperature and pressure are required to achieve sufficient yield. The thermodynamic and kinetic issues can be addressed using an electrochemical cell, which enables the reaction to occur at lowered operating temperature resulting in high conversion and selectivity. Crystalline $SrMoO_4$ anode catalysts synthesized via sol-gel method showed significantly enhanced catalytic performance on the ODH reaction without current in the electrochemical cell with 32 mol% of propylene selectivity, which is 20 % higher than pack-bed reactor at 200 ^{o}C lowered operating temperature. Therefore, we are expecting to get more than 50 mol% of propylene selectivity and more than 30 mol% of propane conversion when current flows into the reactor in the future.

Keywords: Catalysis, Propane ODH, SOEC, Propylene

B.10 Advanced H_2S processing with Coproduction of Hydrogen and Elemental Sulfur Using Thermo-Catalytic Sulfur Capture Process

Presenter: Kalyani Jangam
Advisor(s): Dr. Liang-Shih Fan
Email: jangam.4@osu.edu
Year of graduation: Summer 2022

Abstract:

Conventional Claus process oxidatively decomposes H_2S stream generated in fuel processing operations into steam and sulfur. However, we have developed thermo-catalytic sulfur capture (TCSC) process for advanced H_2S processing, producing H_2 instead of H_2O by following a non-oxidative decomposition route. The process consists of two primary steps where in the sulfidation step, iron sulfide (FeS) catalytically decomposes H_2S into H_2 and sulfur with latter reacting with FeS, producing sulfur rich phase FeSx (where, x>1). The captured sulfur is then recovered in the regeneration step by thermally decomposing FeSx into FeS at a higher temperature in an inert atmosphere. First-principles density functional theory (DFT) simulations show an improvement in reaction kinetics by addition of dopants in FeS, modifying its surface electronic structure. Fixed bed experiments were performed to corroborate DFT simulation results showing an improvement in H_2S conversion over FeS. Thus, this work offers a cost-effective technology with a potential to replace the conventional H_2S processing scheme.

Keywords: Hydrogen, Iron sulfide, Dopant modification

B.11 Enhanced Dry Reforming of Methane Using a Tailored Metal Oxide(TMO)

Presenter: Pinak Bhushan Mohapatra
Advisor(s): Dr. Liang-Shih Fan
Email: mohapatra.23@osu.edu
Year of graduation: 2023

Abstract:

The challenges in the dry reforming of methane have attracted significant attention by researchers recently. The technology proposes to utilize two greenhouse gases to produce value-added product syngas. However, stable and efficient catalytic material design to prevent carbide and oxide-induced deactivation is still lacking. Also, operating parameters such as temperature and pressure critically influence the product purity and catalyst deactivation. A thermodynamic feasibility study of the methane reforming process with the help of the proposed iron-based tailored metal oxide (TMO)is carried out. Based on the study, a ratio of CO_2:CH_4 higher than one is tested at 1000°C and pressure ranges between 1 to 5 atm to prevent carbon deposition and produce syngas at a stable rate with higher yields for a prolonged time. The analysis of chemistry shows iron-based TMO exhibits different solid phases during the progress of the reaction and has been observed to follow the mechanism similar to methane to syngas chemical looping system. The process addresses the deactivation issues and determines the optimized operating parameters to achieve higher CO_2 and CH_4 conversion.

Keywords: Dry methane reforming, Metal oxide, Syngas

B.12 Gas-phase Hydrodeoxygenation of Phenol over Swellable Organically Modified Silica

Presenter: Anagha Hunoor
Advisor(s): Dr. Umit Ozkan
Email: hunoor.1@osu.edu
Year of graduation: 2022

Abstract:

Lignocellulosic biomass is an excellent feedstock for biofuel production as it is abundant and inedible. However, bio-oil obtained from pyrolysis of this feedstock is rich in oxygenates like phenols, furans, carboxylic acids etc. These compounds impart instability to bio-oil and lower its energy density. Hydrodeoxygenation (HDO) is employed to remove oxygen, in the form of water and improve the properties of bio-oil. NiMo sulfide supported on Al_2O_3 is used as one of the commercial catalysts for HDO. Catalyst deactivation due to water is a major problem associated with sulfide catalysts. In this work, Ni-MoS_2 catalyst supported on swellable organically modified silica (SOMS) was synthesized for HDO of phenol. SOMS is a mesoporous hydrophobic silica-based material. HDO of phenol was carried out in a flow reaction system at 200-300^{o}C under atmospheric pressure. The hydrophobicity of SOMS can prevent the deactivation of our catalyst.

Keywords: Hydrodeoxygenation, Phenol, Gas-phase

B.13 Swellable Organically Modified Silica: A Novel Support for Catalytic Hydrogenation and Hydrogenolysis Reactions in Aqueous Phase

Presenter: Saurabh Ailawar
Advisor(s): Dr. Umit Ozkan
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Year of graduation: Summer 2020

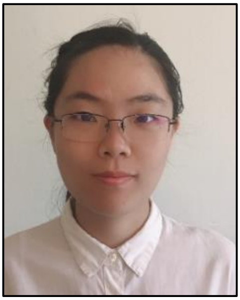
Abstract:

Swellable Organically Modified Silica (SOMS) is a hybrid organic-inorganic material belonging to the class of bridged polysilsesquioxanes. It has high affinity to organic solvents and is highly hydrophobic. In presence of organic solvents, it undergoes swelling, resulting in increased pore size and surface area. This study investigates the role of SOMS as a catalytic support for degradation of organic pollutants in aqueous media.

Hydrodechlorination of trichloroethylene and hydrogenation of toluene, are the model reactions to study 1%Pd/SOMS and 1%Ru/SOMS respectively. During these reactions, ethanol is used to swell SOMS and, its effect on the catalytic activity is discussed. Commercially available Al2O3 supported catalysts are used for comparison. Deactivation resistance of these catalysts in presence of chloride and sulfide species is also investigated. Characterization techniques such as, transmission electron microscopy (TEM), X-ray absorption spectroscopy (XAS), Fourier transform infrared spectroscopy (FTIR) and nitrogen physisorption, are used to study the aspects mentioned above.

Keywords: Catalyst, Silica, Hydrogenation, Pd, Hydrophobic

B.14 Fe_2O_3@SBA-15 as an Efficient and Stable Catalytic Oxygen Carriers for Chemical Looping Partial Oxidation of Methane



Presenter: Yan Liu
Advisor(s): Dr. Liang-Shih Fan
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Year of graduation: 2021

Abstract:

Chemical looping partially oxidation of methane is one the most promising techniques to generate syngas. Developing high performance oxygen carriers are the key to this process. In this research, Fe_2O_3 nanoparticles embedded in mesoporous support SBA-15 (Fe_2O_3@SBA-15) was synthesized and applied to chemical looping partial oxidation to generate syngas. Techniques including XRD, BET, TEM, SEM, and TGA were used to characterize the material before and after reaction. Results showed that Fe_2O_3@SBA-15 have enhanced stability and reactivity, with a conversion rate 70% higher than bulk Fe_2O_3. This can be attributed to tube structure of the support SBA-15, which provides large space and surface area for Fe_2O_3 nanoparticles and prevent the agglomeration of nanoparticles during reaction. In addition, selectivity was also test in TGA. Results showed that very low concentration of CO_2 was observed during reaction, indicating high syngas selectivity >99%. This designed material has the potential to generate pure syngas at relatively low temperature. This study provides guidance on the design of novel oxygen carriers for chemical looping partial oxidation.

Keywords: Catalytic, Methane oxidation, Nanoparticle

B.15 Suppression of coke formation by tailoring the A-site stoichiometry of a lanthanum strontium ferrite cathode during CO_2 electrolysis

Presenter: Dhruba Jyoti Deka
Advisor(s): Dr. Umit Ozkan
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Year of graduation: Spring 2020

Abstract:

The high operating temperature (upwards of 500°C) of solid oxide electrolysis cells makes the adsorption of CO_2 on the cathode surface difficult during CO_2 electrolysis. To enhance CO_2 adsorption on the cathode, an approach is to use an A-site excess perovskite oxide cathode. Another way of enhancing performance for CO_2 electrolysis is controlled exsolution of B-site metal ion from an A-site deficient perovskite host. A-site stoichiometry, therefore, plays an important role in determining the cell performance. However, there has been no study to investigate the impact of such materials engineering on the side reactions such as coke formation. In this study, effect of A-site stoichiometry of a lanthanum strontium ferrite- based perovskite oxide on CO_2 electrolysis is investigated. It was found that while an A-site deficient cathode improves the electrochemical performance for CO_2 electrolysis, an A-site excess cathode reduces the electrochemical activity for CO_2 electrolysis and leads to formation of coke.

Keywords: CO_2 conversion, Perovskite Oxide, SOEC

C.1 Achieving Campus Carbon Neutrality - Applying Sustainable Engineering Methods to Evaluate Technical and Ecological Solutions

Presenter: Michael Charles
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Year of graduation: 2021

Abstract:

Currently, over 300 academic institutions have committed to achieve carbon neutrality before 2100. In response, many institutions focus solely on technological options to reduce emissions, but don’t properly include ecological solutions. What impacts could including nature-based solutions have on campus sustainability in pursuit of carbon neutrality? Further, how do we compare these results with the trade-offs of other technological and behavioral solutions? Optimization methods can be applied to compare the estimated carbon reductions and costs for any number of options, presenting multi-solution (technical and ecological) strategies that meet the University’s needs. Understanding financial, technological, spatial, and social constraints and dynamics of the carbon reduction strategies can inform the optimization problem to assist the development of a university’s action plan to achieve neutrality. This research discusses some of the options and challenges that exist in reaching carbon neutrality for academic institutions, while also demonstrating a potential plan for a large University.

Keywords: Sustainability, Optimization, Business management

C.2 Co-Production of Syngas and Hydrogen Using Calcium-Iron Based Oxygen Carriers for Chemical Looping Reforming Process

Presenter: Vedant Shah
Advisor(s): Dr. Liang-Shih Fan
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Year of graduation: 2021

Abstract:

The work done here focuses on co-production of syngas and high-purity hydrogen using a two-reactor chemical looping system that makes use of calcium ferrite ($Ca_2Fe_2O_5$) as an oxygen carrier and natural gas as fuel. The material used has brownmillerite type structure, thus allowing rapid transport of oxygen ions through the material ensuring excellent reaction kinetics. Assessment of oxygen carrier samples was done using thermogravimetric analyzer (TGA) and fixed bed where they were reduced in methane and oxidized back in steam/CO_2 to complete the loop. Thermodynamic analysis of various reactions involved in the proposed chemical looping system was done to understand the interaction between various gaseous and solid species with each other. Solid samples were characterized using techniques like SEM, EDS and XRD. Thermodynamic analysis and experiments prove that $Ca_2Fe_2O_5$ is an attractive oxygen carrier for methane reforming to produce syngas with >95% purity and achieve ~85% steam conversion.

Keywords: Chemical looping reforming, Brownmillerite

C.3 Experimental Study on the Hydrodynamics of Slugging Fluidized Bed with Electrical Capacitance Volume Tomography

Presenter: Yaswanth Pottimurthy
Advisor(s): Dr. Liang-Shih Fan
Email: pottimurthy.1@osu.edu
Year of graduation: 2020

Abstract:

With recent advances in the sensor development and image construction techniques for the electrical capacitance volume tomography (ECVT) for 3-D multiphase flow imaging, it is now possible to use the ECVT to obtain the reconstructed 3-D image of multiphase flow phenomena in real time. In this study, three-dimensional ECVT sensors were applied to imaging the flow structures of gas-solids slugging fluidized beds. The detailed 3-D images were obtained and analyzed to reconstruct the real time 3-D gas-solids volume fraction profile of the bed. The entire evolving process of the slugging fluidization from its formation to breakage was analyzed. The solids volume fraction profiles of the slugging bed were plotted under different gas velocity conditions. Particles with different sizes were used in the experiments to investigate the different hydrodynamic characteristics of round-nosed and square-nosed slugging beds.

Keywords: Gas solid flows, Slugging fluidization, ECVT

C.4 Homogeneous Hydrodynamics in an Evolving Granular Fluid

Presenter: Qiaochu Zhang
Advisor(s): Dr. Liang-Shih Fan
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Year of graduation: 2023

Abstract:

In this study, the hydrodynamic property of the granular system is studied by comparison of results from Enskog equation and molecular dynamics simulation to show potential directions of improvement for kinetic theory. The kinetic theory has been proposed to describe the granular system with some drawbacks such as the intricacy in solving Enskog kinetic equations and limitation in the assumptions of the system. In order to further understand the granular system, a molecular dynamics simulation is conducted for a three-dimensional freely evolving inelastic granular gases in homogenous cooling state. Evolutions of granular temperature and Sonine coefficient a2 are compared with theoretical results. Discussions are conducted about these results and suggestions for future modification of kinetic theory are put forward.

Keywords: Kinetic theory, Granular flow

C.5 Towards Circular Economy: determining optimum pathways for enabling Sustainable Life-cycle of Plastic grocery bags.

Presenter: Vyom Thakker
Advisor(s): Dr. Bhavik Bakshi
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Year of graduation: 2023

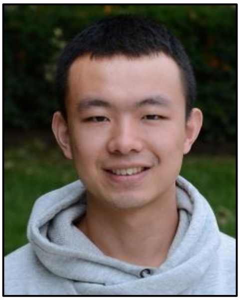
Abstract:

Plastics are accumulating at an alarming rate into the ecosystems as pollutants and waste, thereby depleting natural capital and causing adverse environmental impact. We propose to make the linear economy of plastics circular using pathway design. This study uses principles of life-cycle assessment and product management, to create a holistic design problem for the pathways involving 5 different makes of grocery bags. These pathways are segregated into the following segments (modelled separately): manufacturing, consumption, disposal and collection, reprocessing, waste treatment, downscaling and end of life. For various objectives including degree of circularity, economic value and global warming potential, the following decisions are made : ratio in which respective plastic bags are consumed, best collection method, appropriate waste management strategy and inevitable losses to environment. This work, therefore guides producers, consumers and policy makers by aggregating and linking decision variables across all segments in the multi-objective non-linear optimization problem.

Keywords: Life-Cycle Design, Circular Economy, Optimization

D.1 CO_2-Selective Membranes for H_2 Utilization Enhancement of Solid Oxide Fuel Cells

Presenter: Kai Chen
Advisor(s): Dr. W. S. Winston Ho
Email: chen.4808@osu.edu
Year of graduation: 2020



Abstract:

Polymeric membranes with a high CO_2/H_2 selectivity are desired to recover H_2 from the anode exhaust of a high-temperature solid oxide fuel cell (SOFC) system for H_2 utilization. The membranes studied contained a polyelectrolyte with fluoride as the counter ion, which catalyzed the reaction between CO_2 and water. The composition also included a boric acid to further catalyze the reaction, and quarternary ammonium-based mobile carriers were employed for the facilitated transport of CO_2. A CO_2 permeance of 100 GPU and a CO_2/H_2 selectivity of 116 at 120 °C were demonstrated. The thermal stability of the quarternary ammonium-containing components was also quantified.

Next, a high-level techno-economic analysis was conducted for the integration of the membrane process into the SOFC system. The effect of membrane transport performances, H_2 recovery, and feed to sweep flow ratio were studied. The CO_2 removal cost using the membrane mentioned above was calculated to be $62.8/tonne.

Keywords: Membranes, CO_2/H_2 separation, Fuel cells

D.2 Carbon Particulate Assisted Extrusion Foaming of Polyethylene Terephthalate (PET) for Thermal Insulation Applications

Presenter: Junjie Pan
Advisor(s): Dr. L. James Lee
Email: pan.687@osu.edu
Year of graduation: 2021

Abstract:

Medium-density PET foams (~ 0.5 g/cm3) were obtained from non-modified semi-crystalline PET resin by a lab-scale twin-screw extruder with a physical blowing agent (HFC134a). The foam morphology was manipulated by micrographite (mGr) and multiwall carbon nanotube (MWCNT) which enhanced the rheological behavior and non-isothermal crystallization kinetics of PET. Low-density PET foams (< 0.15 g/cm3) was also produced by manipulating the PET molecular weight by in-situ moisture-induced controlled-hydrolysis. Moisture-contained activated carbon (AC), which allowed easier control of the moisture content, decreased the resin molecular weight to an acceptable level without losing crystallinity, and thus the PET foams possess better tensile properties (~2 MPa stress and ~100% strain) and higher thermal stability (>200°C) than chemically modified PET foams. A strand array die was also designed to produce plate-shaped foam samples. Both AC and mGr stabilized the foam morphology and served as good infrared attenuation agents (IAAs) in a simulated housing thermal insulation experiment.

Keywords: PET, Extrusion foaming, Carbon particulates

D.3 Structure of Segmented Ionenes Containing Spherical Nanoparticles

Presenter: Nicholas Liesen
Advisor(s): Dr. Lisa Hall and Dr. Isamu Kusaka
Email: liesen.3@osu.edu
Year of graduation: 2021

Abstract:

Polymer nanocomposites are versatile materials in which composition of the polymer matrix, NP size and chemical properties, and presence or absence of ionic groups can be manipulated to optimize material properties for various applications. Designing these materials is challenging due to the multiple length scales involved and tendency of NPs to aggregate in the polymer matrix, depending on the polymer-NP interactions. Thus, efficient coarse-grained simulation methods are appropriate as they can access the monomer and particle length scales, as well as the time scales of polymer relaxation and adsorption/desorption on the NP.

In this work coarse-grained molecular dynamics simulations are used to explore the structure and dynamics of multiblock ionomers with free counterions and added spherical NPs. Experimental work, which synthesized a variety of such ionomers with different block lengths and compositions, suggests a promising route to controlling material properties. In simulation, we tune similar parameters, adjust NP chemistry, and find local microphase segregation of soft and hard polymer blocks without long range order. Parameters are suggested to improve NP dispersion.

Keywords: Polymer nanocomposites, Nanoparticles, Simulation

D.4 Amine-Containing Mixed-Matrix Membranes Incorporated with Amino-Functionalized Multi-walled Carbon Nanotubes for CO_2/H_2 Separation

Presenter: Yutong Yang
Advisor(s): Dr. W. S. Winston Ho
Email: yang.4249@osu.edu
Year of graduation: 2022

Abstract:

Syngas, consisting of mainly H_2 and CO_2, needs to be separated to complete the conversion of CO and obtain high purity H_2, which can act as a clean, renewable fuel gas for widely commercial uses. Mixed-matrix membrane is with incorporated nanofillers containing CO_2 carriers is one kind of facilitated transport membrane, which shows remarkable transport performance and excellent stability operated under high pressures and high temperature. In the present work, amino-functionalized multi-walled carbon nanotubes (AF-MWNTs) were chosen as the mechanical reinforcing filler to enhance the membrane stability and as the CO_2 carrier to facilitate CO_2 transport. Variable amounts of AF-MWNTs were incorporated to crosslinked PVA-poly(siloxane)/amine membranes to synthesize the CO_2-selective mixed-matrix membranes. The membrane containing 10 wt.% MWNTs demonstrated optimal stable CO_2 permeability of 1090 Barrer and CO_2/H_2 selectivity of 48 for the 100-h test at 1.5 MPa and 107 °C. The primary purpose of this work was to investigate out the effect of AF-MWNTs loading in the mixed-matrix membrane under high pressure in order to obtain the optimal transport performance.

Keywords: Mixed-matrix membrane, Multi-walled carbon nanotubes

D.5 Computational Investigation of Zeolite Nanosheets as Pervaporation Membranes for Ethanol Extraction

Presenter: Changlong Zou
Advisor(s): Dr. Li-Chiang Lin
Email: zou.153@osu.edu
Year of graduation: 2021

Abstract:

To accelerate the development of green energy (i.e., ethanol) to meet the increasing demand of global energy with less CO_2 emission, state-of-art molecular dynamics methods are employed in this study to explore the separation performance of novel 2-dimensional materials, zeolite nanosheet membranes, for the investigation of key factors that determine the separation performance. A diverse set of zeolite nanosheets are studied and show tremendous flux compared to the currently available membranes. However, the separation factors can vary dramatically from 6.67 to 440. To better understand the reasons behind the large difference between the separation factors, the adsorption selectivity, surface/entrance ethanol fraction, and their combinational effects are studied. Also, structural properties that affect the entrance ethanol fraction have been identified. Moreover, the total flux is shown proportional to the density and the size of the channels. Overall, in this study, correlations between the separation performance and their structural features are established and can be used to identify the promising membrane candidates from databases in a large-scale screening study.

Keywords: Nanosheet, Zeolite, Pervaporation, Simulation

D.6 Understanding Polymeric Facilitated Transport Membranes for Post-Combustion Carbon Capture at a Molecular Level

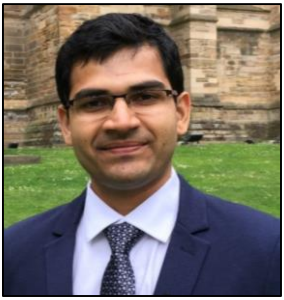
Presenter: Xuepeng Deng
Advisor(s): Dr. Ho and Dr. Li-Chiang Lin
Email: deng.465@osu.edu
Year of graduation: 2021

Abstract:

Polymeric facilitated transport membranes (FTMs) are attracting growing attention for their promising separation performance in post-combustion carbon capture. Different from traditional polymeric membranes, FTMs contain amines that selectively react with CO_2 and thus provide an alternative of CO_2 transport mechanism to the solution-diffusion mechanism. The advancement of modern computational techniques, such as molecular dynamics (MD), Monte Carlo (MC), and density functional theory (DFT), provides opportunities to study FTMs and understand their separation performance at a molecular level. In this study, these methods are employed to investigate the reaction mechanisms, morphology, and permeation behaviors of FTMs of different compositions. The molecular-level insights obtained offer a theoretical interpretation of the experimentally observed behaviors of FTMs, and the outcomes of this study are anticipated to expedite the search for FTMs with enhanced separation performance.

Keywords: Facilitated transport membrane, Carbon capture

E.1 Surface Area Determination of Porous Materials



Presenter: Archit Datar
Advisor(s): Dr. Li-Chiang Lin
Email: datar.10@osu.edu
Year of graduation: 2020

Abstract:

Porous materials have been shown to be promising for use in several environmental applications such as storage of natural gas in natural gas-powered vehicles, capturing water from air, etc. Some of their most important performance parameters for these applications are dependent on their accessible surface area. Thus, the determination of the accessible surface area is an important step in the screening of materials for an application. Traditionally, the BET method has been used for this purpose. However, it has been found that, in some cases, the BET surface area might not be a good representation of the actual accessible surface area. In this study, we discuss the limitations of the BET method and propose ways to supplement it, in order to provide a more accurate surface area prediction.

Keywords: Porous materials, BET theory, Surface area

E.2 Encapsulation of Hydrophobic Drugs in Polymeric Nanoparticles Using Electrohydrodynamic Mixing Mediated Nanoprecipitation

Presenter: Faiz Khan
Advisor(s): Dr. Jessica Winter
Email: khan.788@osu.edu
Year of graduation: 2023

Abstract:

Hydrophobic drugs are poorly soluble in biological environment, limiting their stability, circulation time, bioavailability and efficacy. Drug delivery systems must provide enhanced solubility of drug with minimal toxicity. Nanoparticles based delivery systems offer a promising way to satisfy pre-requisites for a delivery system but also to provide added advantages including high drug loading, controlled and stimuli-responsive smart release. Amphiphilic block copolymers can be used for encapsulation of drug inside hydrophobic core with hydrophilic corona providing stabilization in an aqueous environment. Despite ongoing efforts, scalable and high throughput synthesis of drug nanoparticles has been limited to flash nanoprecipitation achieved through jet mixers employing confined geometries. Recently developed, Liquid in Liquid electrospray system provide a facile step towards nanoparticle development. Herein, we report the encapsulation and characterization of drugs such as coumarin-6, dexamethasone, lutein and vorinostat (SAHA) in polycaprolactone-b-poly(ethylene oxide) and polystyrene-b-poly(ethylene oxide) block copolymer nanoparticles.

Keywords: Nanoparticles, Electrospray, Block copolymer

E.3 Size, Structure, and Phase of Carbon Dioxide Aerosols formed by Homogenous Nucleation

Presenter: Kayane Dingilian
Advisor(s): Dr. Barbara Wyslouzil
Email: dingilian.1@osu.edu
Year of graduation: 2021

Abstract:

Supersonic separation is a promising technology for application to carbon capture. Understanding and characterizing the mechanism of the nucleation of carbon dioxide (CO_2) is crucial for the successful implementation of supersonic separation. We used Fourier transform infrared (FTIR) spectroscopy measurements to characterize the size, structure, and shape of the condensed CO_2 particles. In particular, we focused on the I3 fundamental vibration peak. Analysis of these spectra suggest an evolution from the gas phase to solid phase as the CO_2 particles condensed. We observed the gas-phase Î3 band centered at 2349 cm^{-1}. In the condensed phase, the Î3 peak shifts to 2359 cm^{-1} with a shoulder at 2360 cm^{-1}. Ongoing collaborations with molecular dynamics and spectroscopy simulation groups provide insight on the shape and structure of the CO_2 particles as they evolve from the gas to condensed phase.

Keywords: Carbon capture, Infrared, Spectroscopy, Aerosols

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