



11th Annual Graduate Research Symposium 2022

Sponsored by The Dow Chemical Co.



Abstract Book



William G. Lowrie Department of

**Chemical and
Biomolecular Engineering**



William G. Lowrie
Department of Chemical and Biomolecular Engineering
11th Annual
Graduate Research Symposium 2022

Sponsored by The Dow Chemical Co.

Keynote Speaker

Sravana Karnati

Senior Vice President

Walmart International Technology



Sravana has over 25 years of leadership experience delivering innovative technology solutions for a variety of industries including retail, travel, media, high-tech and chemical.

Sravana currently serves as the Senior Vice President of Technology for Walmart International. His team develops solutions for everything from POS to eCommerce to power a \$100B+ business

spanning across 5,200+ stores and 550,000+ associates in 23 countries.

Prior to that, Sravana served as the Chief Product and Technology Officer for Sterling, a leading provider of background screening and identity services. Sravana also held leadership roles at Egencia, Disney, Amazon, Oracle and other companies.

Sravana holds a doctorate in AI Applications in Chemical Engineering from The Ohio State University, a Master of Technology degree in Chemical Engineering from Indian Institute of Technology, Madras and a Bachelor of Technology degree in Chemical Engineering from Anna University, Madras.

He and his wife are originally from Chennai, India, and have two children.



Event Schedule

11th Annual GRS

Friday September 23rd, 2022

Time	Event	Location
8:00 – 8:30 am	Registration & Breakfast	Grand Lounge
8:30 – 8:45 am	Opening Remarks	Grand Lounge
8:45 – 9:30 am	Keynote Address	Grand Lounge
Break		
9:45 – 11:00 am *	Oral Presentations Session 1	Grand Lounge
Break		
11:15 – 12:30 pm *	Oral Presentations Session 2	Grand Lounge
12:30 – 2:00 pm	Lunch & Networking	Main Dining Room
2:00 – 4:00 pm	Poster session	Main Dining Room
4:15 – 4:30 pm	Closing Remarks & Award Session	Main Dining Room
4:30 – 5:00 pm	Reception & Networking	Main Dining Room

*Oral presentations: 15 minutes total
(12 for presentation, 3 for questions)

List of Attendees

Category: Industry Representatives/Alumni

Name	Company
Dan Coombs	Independent
Wendy Flory	Dow
Rick Watson	LyondellBassel
Zhang Liping	Dow
Edward Marzal	Kenexis
Anna Opella	Dow
You Peng	Dow
Adam Pitz	P&G
Michael Triplett	Carmen Ventures



Session 1

Oral Presentations

Friday September 23rd, 2022

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10:00- 10:15 am	Enrichment of aged and sickled red blood cells based on Hb content and saturation using permanent magnets and annular flow Mitchell Weigand	4
10:15- 10:30 am	Aqueous phase hydrodechlorination of trichloroethylene using Pd supported on swellable organically modified silica (SOMS): Effect of support derivatization Anagha Hunoor	5
10:30- 10:45 am	Exploring the potential of Ni₃S₂ based sulfur looping process for efficient production of H₂ from H₂S Anuj Joshi	6



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Oral Presentations

Friday September 23rd, 2022

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11:45- 12:00 pm	Microfluidic harvesting of breast cancer tumor spheroid-derived extracellular vesicles from immobilized microgels for single-vesicle analysis Xilal Rima	9
12:00- 12:15 pm	Insights into electrochemical bromine evolution reaction (BER) active sites for nitrogen-doped carbon nanostructures (CN_x) Dishari Basu	10



Upgrading biomass through the aldol condensation using cooperative interactions in aminosilica materials: Discovering the different types of catalytic sites in aminosilica materials

Presenter: Jee-Yee Chen

Advisor: Dr. Nicholas Brunelli

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Year of graduation: 2023



Abstract:

Biomass upgrading to chemicals and fuels requires development of highly active and selective catalytic materials for important reactions, including aldol chemistry. Aldol chemistry can be catalyzed by powerful enzymes employing cooperative interactions between acids and bases to form C-C bonds. Translating cooperative interactions into heterogeneous catalysts such as aminosilicas is beneficial to create highly active and reusable catalysts. Interestingly, previous work for aminosilicas has assumed that each amine site is equivalent, but this assumption has not been rigorously tested. This work demonstrates that multiple types of amine sites exist, and the relative amount of each site can be tuned through controlling synthesis parameters, specifically surface density. For standard aminosilica materials with micropores (REG), only 30% of the overall sites are active through site quantification. By synthesizing reduced micropore volume materials (NMP), the fraction of active sites can increase to 50%. The NMP materials have more than double the catalytic activity of the REG materials. Importantly, we discover that there are multiple active sites, and the difference between materials activity can be attributed to the different fraction of the sites. As multiple sites exist, investigating synthesis-structure-function behavior, including the effect of surface density, is important. As surface density increases, it's likely that more cooperative amine-silanol interactions would be disrupted, impacting the active site distribution. Through decreasing the surface density, we increase the fraction of highly active sites. Overall, the work provides new insights on the different types of catalytic sites in the aminosilica materials and provides a direction for future advances.



Enrichment of aged and sickled red blood cells based on Hb content and saturation using permanent magnets and annular flow

Presenter: Mitchell Weigand

Advisor: Dr. Jeffrey Chalmers

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Year of graduation: 2022



Abstract:

Approximately 36,000 units of red blood cells (RBCs) are used every day in the U.S. and approximately 10 million of the 13.6 million collected RBC units are used in the United States. This small surplus of RBCs does not reflect day-to-day inventory nationwide or the challenge of matching donor and recipient blood types. In 2015, approximately 668,000 units outdated in blood centers and hospitals due to the FDA's 42-day storage limit. Although a typical recipient rejects 25% of the transfused cells at this point in storage, many functional RBCs remain. Additionally, large amounts of donor blood that are used to treat symptoms of sickle cell disease (SCD) are wasted during exchange transfusions.

Magnetic fractionation is a promising technology to reduce this waste by isolating the healthy RBCs from aged or sickled cells. By exploiting the magnetic characteristics of paramagnetic, iron-containing Hb, a permanent quadrupole magnet (QMS) is used to exert a differential magnetic force on RBCs based on the quantity and magnetic susceptibility of its Hb. Inside the QMS, one and two phase mixtures flow through an annulus under low Reynolds numbers and a high magnetic field gradient (286 T/m) that causes the deflection of the Hb-rich RBCs from their original path and into an enriched outlet. Our results demonstrate that although the outlet populations have significant differences in Hb content and oxygen affinity, there exists a tradeoff between throughput and purity. These challenges can be addressed with changes to buffer and creative instrumentation.



Aqueous phase hydrodechlorination of trichloroethylene using Pd supported on swellable organically modified silica (SOMS): Effect of support derivatization

Presenter: Anaha Hunoor

Advisor: Dr. Umit S. Ozkan

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Year of graduation: 2023



Abstract:

Hydrodechlorination using Pd catalysts is an effective approach to convert TCE present in groundwater, into benign products, ethane and HCl. However, HCl formed during the reaction deactivates conventional Pd/Al₂O₃ catalysts. This prompted development of deactivation-resistant HDC catalysts. Our group reported the superior deactivation resistance of Pd supported on a novel animated material known as swellable organically modified silica (SOMS). SOMS is a hydrophobic organic-inorganic hybrid material with a high affinity for organics and an ability to swell on exposure to organics. In this study, we investigated the high deactivation resistance of Pd/SOMS to HCl to determine if it was due to hydrophobicity of SOMS or swellability or a combination of both. To that end, samples with varying degrees of hydrophobicity and swellability were synthesized by changing the extent of surface derivatization during sol-gel synthesis of SOMS. The impact of surface derivatization on hydrophobicity, swellability and surface area was confirmed by infrared spectroscopy and N₂ physisorption. After Pd impregnation, the particle size, location, and atomic environment of Pd were also found to be governed by support derivatization. The sample with no derivatization provided lowest protection to Pd from HCl. To study the interaction of HCl with Pd, pristine catalysts were treated with HCl solutions. For these HCl-treated samples, batch activity rate constants decreased by 66% for the least derivatized sample and 17% for the most derivatized one, suggesting that hydrophobicity and swellability are essential for obtaining high resistance to HCl which could potentially impact the economic viability of HDC of TCE.



Exploring the potential of Ni_3S_2 based sulfur looping process for efficient production of H_2 from H_2S

Presenter: Anuj Joshi

Advisor: Dr. Liang-Shih Fan

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Year of graduation: 2023



Abstract:

Hydrogen Sulfide (H_2S) is a toxic gas released during the processing of fossil fuels. Current projections estimate that hydrocarbon fuels are slated to dominate energy production until 2050. Thus, a high amount of H_2S generation is expected for the next couple of decades, making its treatment critical. Claus process, the state-of-the-art H_2S abatement technology, is ineffective in extracting value from H_2S , as it converts the ‘Hydrogen’ content of H_2S into low-value steam instead of valuable hydrogen (H_2). To counter this, a sulfur looping process scheme utilizing Ni_3S_2 as a sulfur carrier was established for decomposing H_2S into H_2 and S. It involves two sub-steps – sulfidation and regeneration. In the sulfidation step, Ni_3S_2 reacts with H_2S forming NiS and H_2 , and in the subsequent regeneration step, sulfur is recovered by thermally decomposing NiS back into Ni_3S_2 in presence of CO_2 . Zirconium oxide (ZrO_2) was used as support to overcome the thermal instability of Ni_3S_2 while providing effective dispersion. The supported sulfur carrier exhibited stable reactivity over 10 continuous redox cycles. Results from density functional theory calculations indicate that ZrO_2 serves as bi-functional catalytic support that increases surface area and participates in H_2S decomposition. The scheme was also demonstrated at a laboratory scale fixed bed reactor, wherein $\sim 80\%$ H_2S conversion was achieved. Moreover, system-level ASPEN thermodynamic analysis revealed that sulfur looping has $\sim 19\%$ higher energy and $\sim 8\%$ higher exergy efficiency compared to the Claus process. The findings from this study can be leveraged to develop an economically attractive and environmentally sustainable process.



Guiding eco-innovations to transition towards a sustainable circular economy with net-zero emissions

Presenter: Vyom Thakker

Advisor: Dr. Bhavik R. Bakshi

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Year of graduation: 2023



Abstract:

Given the urgency of action towards mitigating climate change and reducing material consumption, there are a plethora of innovative technologies, supply-chains and policy-actions being proposed. These are targeted towards reducing direct emissions and natural resource uptake. Recently, circular innovations are also being proposed to decouple technological systems from fossil-based 'linear' economies. It is essential to screen these alternatives based on potential for improving the current product value-chains (from resource extraction to end-of-life) through direct implementation and synergies. Once a manageable subset of innovations is screened, it is of growing interest within industries and governments to rank these 'eco-innovations' based on their scope of adoption and achieving a sustainable and circular value-chain. As part of this work, we have developed a novel methodology to meet these needs, which relies on multi-objective optimization of life-cycle networks to screen and rank eco-innovations. This method is demonstrated for transforming the Grocery bags' value-chain through plastic packaging innovations, compiled by our collaborators at the Global Kaiteki Center. The screening step identifies hotspots and sensitive activities of the value-chain, thereby guiding future research and development in critical sectors using anticipatory LCA models. Further computation yields an eco-innovation ranking from over 150 innovations based on a quantitative win-win criteria, and an assessment of the screened eco-innovations to achieve a net-zero carbon economy with up-cycling. Therefore, this work provides a decision-making framework to climate investors, corporate R&D and policy-makers, for helping them plan sustainability transitions and achieve lofty climate-change and circularity pledges enterprises have made for the future.



***In-situ* exsolution of bimetallic CoFe nanoparticles on (La,Sr)FeO₃ perovskite: Its effect on oxidative coupling of methane**

Presenter: Jaesung Kim

Advisor: Dr. Umit S. Ozkan

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Year of graduation: 2023



Abstract:

Refinement of shale gas over the past several decades has produced an abundance of methane that is typically wasted by the practice of gas flaring. One strategy is to use a membrane reactor for OCM operating at low partial pressures of oxygen. A further advantage of solid oxide cells is that electricity can be spontaneously generated during OCM. We explored La_{0.7}Sr_{0.2}Co_{0.2}Fe_{0.8}O₃ (LSCF) catalyst as an anode for oxidative coupling of methane to ethylene and propylene. LSCF underwent the structural transformation under 5% H₂/N₂ at 850°C as demonstrated by XRD. The main XRD peaks of LSCF remained after 1 h of reduction at 850°C (H₂-Red-LSCF), but the additional features corresponding to bimetallic CoFe, LaSrFeO₄, and La₂O₃ also emerged. Moreover, XRD analysis showed that the CH₄-treated LSCF (CH₄-Red-LSCF) experienced the same structural transformation as H₂-Red-LSCF, displaying peaks present in CoFe alloy and LaSrFeO₄. TPD-DRIFTS using CO₂ as a probe molecule were conducted on LSCF and Red-LSCF, and the results verified that the surface of Red-LSCF is more basic than that of LSCF and that reduction is an effective way of promoting the catalytic characteristics of LSCF for the activation of CH₄. Moreover, in order to gain insight into the surface dynamics during CH₄ activation, *in-situ* CH₄-DRIFTS measurements were conducted on LSCF and Red-LSCF catalysts under CH₄ atmosphere at 450°C. According to the results, CH₄ coupling reaction to C₂₊ is competing with the oxidation of CH₄ and the controlled oxygen supply is a key parameter for a selective conversion of CH₄ on Red-LSCF.



Microfluidic harvesting of breast cancer tumor spheroid-derived extracellular vesicles from immobilized microgels for single-vesicle analysis

Presenter: Xilal Rima

Advisor: Dr. Eduardo Reátegui

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Year of graduation: 2023



Abstract:

Investigating cellular and vesicular heterogeneity in breast cancer remains a challenge, encouraging the engineering of controllable *in vitro* systems. Microgels afford identical isotropic conditions for tumor growth but are compromised by the adversity of fluid exchange. Therefore, we developed monodisperse three-dimensional extracellular vesicle (EV) microbioreactors ($^{EV}\mu\text{BRs}$) to model micrometastatic EV release and a novel method to immobilize the $^{EV}\mu\text{BRs}$ within a microchannel to harvest the EVs. Flow-focusing droplet generation enabled the rapid production of identical $^{EV}\mu\text{BRs}$ with a coefficient of variation of 1.73 ± 0.46 % that were tunable for diameter and cellular occupancy. The $^{EV}\mu\text{BRs}$ supported the growth of tumor spheroids, which demonstrated phenotypic heterogeneity. Two-layer hydrodynamic traps were polymerized *in situ* with a digital-micromirror-device-based UV projection system in less than 15 min, outperforming current soft-photolithographic techniques. The hydrodynamic traps immobilized the $^{EV}\mu\text{BRs}$ via a locking mechanism at an efficiency of 94.17 ± 6.97 %. Spheroid-derived EVs could be harvested with as little as ~ 20 μL from the microchannel. The majority of the spheroid-derived EVs were small EVs, which demonstrated a heterogenous expression of tetraspanin proteins. The $^{EV}\mu\text{BRs}$ were loaded with various densities of cells whereby the secretion of EVs across the various densities was analyzed via tunable resistive pulse sensing from suspended $^{EV}\mu\text{BRs}$ and single-EV immunofluorescence from the microfluidic system, where both quantification methods coincided in determining a density-dependent increase in EV production. The platform affords a facile, reliable, tunable, and quantifiable method to investigate micrometastatic EV release, which can be translated to other three-dimensional disease models.



Insights into electrochemical bromine evolution reaction (BER) active sites for nitrogen-doped carbon nanostructures (CN_x)

Presenter: Dishari Basu

Advisor: Dr. Umit S. Ozkan

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Year of graduation: 2023



Abstract:

Recently, electrochemical halide oxidation processes have garnered much attention to replace commercial methods for halogen production. Currently, large scale bromine manufacturing requires transportation and handling of hazardous chlorine gas as the bromide oxidant making this process unsafe, thereby creating a need for a novel approach for bromine evolution. The traditional electrochemical bromine production process involves bromine evolution reaction (BER) on the anode while hydrogen evolution reaction (HER) occurs on the cathode. However, the anode catalysts are generally platinum or graphitic carbon which is an expensive noble metal or leads to sluggish reaction kinetics respectively. To that end, we report nitrogen-doped carbon nanostructures (CN_x) as robust platinum group metal free electrocatalysts for BER. CN_x showed higher current densities than 10% Pt/C even at low bromide concentration at low overpotentials. It was also found to be stable under high oxidative potentials up to 18 hours without carbon corrosion in the presence of dissolved bromide ions. CN_x catalysts contain various types of active sites which have been revealed using density functional theory (DFT) calculations in conjunction with experimental X-ray Photoelectron Spectroscopy (XPS). These characterization studies are used to elucidate the nature of BER active sites and propose the BER mechanism occurring over CN_x. This work demonstrates the applicability of CN_x as a promising noble metal free electrocatalyst for bromine production at room temperature and may be used as a guide to tailor active sites on similar class of catalysts in future for more cost-effective bromine evolution.



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A.1 DNA-caged polymer micelles for cell and tissue labeling

Presenter: Elizabeth Jergens

Advisor: Dr. Jessica Winter

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Year of graduation: 2022



Abstract:

Standard pathology is used every day to diagnose individuals with a variety of conditions, especially cancer. The main difficulty with this method is the limited number of biomarkers of interest that can be observed in each tissue slice and the permanent nature of the stains. More labels per sample would offer more complex pathway analysis and therefore more accurate diagnosis. Here we propose erasable labels using DNA caged polymer micelles. Standard DNA binding rules allow for easy duplex formation between complimentary strands and then replacement of one strand with a more complimentary strand. Thus far, DNA caged polymer micelles have shown promise as erasable labels in solution, on slides, and in fixed cells. Erase depth and tissue penetration studies have also been conducted as progress towards using DNA cages in the standard pathology workflow has been made. Future work will focus on labeling of multiple targets in different colors as well as labeling tissue slices.

A.2 Exploring the impact of exteins on the C-terminal cleaving kinetics of Δ I-CM inteins

Presenter: Hongyu Yuan

Advisor: Dr. David Wood

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Year of graduation: 2023



Abstract:

In the downstream protein process, it is a very common method to add tags to proteins to achieve corresponding functions, so the problem of how to remove tags has also been greatly developed. The intein-based self-cleaving system is one solution to this problem. The Δ I-CM intein has been widely used in self-cleaving tag systems due to the advantages of its small size and pH sensitivity. To construct a self-cleaving tag system, the target protein is usually connected to the C-terminus, and the affinity tag is connected to the N-terminus. However, the C-terminal cleaving rate is still not satisfactory. A lot of research on the mechanism of intein cleaving activity suggests that the extein residues have a significant impact on its cleaving kinetics. To optimize the Δ I-CM intein-based self-cleaving tag system and promote the analysis of the Δ I-CM intein's cleaving activity, this research aims to detect if and how the extein residues affect the cleaving rate of the Δ I-CM intein. The cleaving kinetics of inteins at different pH with different extein residues were detected. The preliminary work has demonstrated that at the appropriate pH, the +1/-1 extein residues have significant impacts on the cleaving kinetics, and that cleavage is controllable by changing the pH.

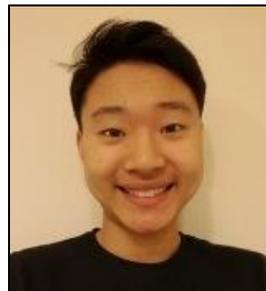
A.3 3D biomimetic hyaluronic acid/collagen hydrogels for *in vitro* modelling of glioblastoma

Presenter: Paul Lee

Advisor: Dr. Jessica Winter

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Year of graduation: 2025



Abstract:

Glioblastoma multiforme (GBM) is the most malignant and common form of astrocytoma with poor prognosis. Treatment with surgery and adjuvant chemo- or radiotherapy is insufficient due to tumor recurrence rates of ~90% which lead to median survival times of 15 months and 5-year survival rate of only ~5%. GBM is unique in that it spreads insidiously with unclear tumor borders, is highly heterogeneous, rarely metastasizes, and takes place in the context of the blood-brain barrier. As such, it has been difficult to understand GBM biology and to develop improved treatments. For improved disease modeling, we have developed a 3D *in vitro* tumor spheroid model using hyaluronic acid and collagen to mimic native brain tissue. With this model, we can recreate an extracellular matrix environment to observe morphologies and migration patterns of GBM in a spatiotemporal manner. Co-localization of GBM cells with normal astrocyte cells further allows us to look at interaction effects as astrocytes and GBM cells are known to engage in crosstalk. Whereas it has been reported that astrocytes can be activated by GBM to become tumor-promoting, we have observed that the presence of astrocytes reduce the migratory capability of GBM cells from the U87 cell line. We will perform RNA extraction and use a tumor signaling panel to observe gene expressions of GBM with and without astrocytes for improved understanding of GBM biology.



A.4 Single step purification of recombinant protein therapeutics using split intein chromatography

Presenter: Sai Vivek Prabhala

Advisor: Dr. David Wood

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Year of graduation: 2024



Abstract:

The therapeutic biopharmaceuticals market has seen tremendous growth over the past few decades as new biologics including recombinant proteins, monoclonal antibodies and gene therapies curing debilitating diseases such as arthritis, hepatitis, melanoma, sarcoma etc. have been commercialized. These biologics are currently being manufactured at high titers using different hosts such as Chinese hamster ovary (CHO) cells, Human embryonic kidney cells (HEK293), *S. cerevisiae* and *E. coli*. Significant challenges exist in the capture and purification of recombinant protein therapeutics due to the lack of scalable platform technologies like Protein A affinity chromatography for monoclonal antibodies. Recombinant protein therapeutics have traditionally been purified using multiple ion exchange, hydrophobic interaction, mixed mode, and ceramic hydroxyapatite chromatography columns. These multicolumn approaches are not selective and often result in low product yields and recovery. In this work, we demonstrate the use of a novel pH sensitive split intein chromatography method for the single step purification of a panel of commercial recombinant protein therapeutics including single chain variable fragment (scFv), Interferon alfa 2b and the receptor binding domain of SARS-CoV2 spike protein. Using this method, we were able to capture and isolate highly pure tagless protein with intact native termini from the cell culture supernatant with high clearance of process and product related impurities such as host cell proteins, host cell DNA, aggregates, chromatin, leached ligand etc. Based on these initial results, we propose the use of iCaptag™-based split intein chromatography as a universal capture platform technology for diverse classes of recombinant therapeutic proteins.



A.5 Zeolitic imidazolate framework–8 encapsulated hemoglobin as a red blood cell substitute

Presenter: Tanmay Nagesh Salvi

Advisor: Dr. Andre Palmer

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Year of graduation: 2026



Abstract:

Hemoglobin (Hb)-based oxygen carriers (HBOCs) have been extensively studied as red blood cell (RBC) substitutes to treat traumatic injuries where the loss of blood causes an oxygen-deficient environment for tissues. Low-molecular-weight HBOCs (~5 nm in diameter) are prone to extravasation through the vascular endothelium, eliciting vasoconstriction, systemic hypertension, and oxidative tissue injury. Zeolitic imidazolate framework- 8 (ZIF-8) is a subclass of metal organic framework (MOF), having zinc as the metal ion and 2-methylimidazole as the organic linker. MOFs are being used in gas separations, catalysis, and drug delivery. For drug delivery applications, ZIF-8 serves as a thermo-stable coating that could increase particle size and enhance the drug's half-life. We have previously synthesized and characterized ZIF-8-bovine Hb (ZIF-8P-bHb) nanoparticles with a diameter of ~100 nm, which avoids the size-related issues mentioned above. In this work, we have synthesized ZIF-8-human Hb (ZIF-8-hHb) nanoparticles with a diameter of ~120 nm and are currently working on purifying and characterizing the oxygen delivery properties of the nanoparticles.



A.6 Sustained release of heme-albumin as a potential novel therapeutic approach for age-related macular degeneration

Presenter: Megan Allyn

Advisors: Dr. Katelyn Swindle-Reilly and Dr. Andre Palmer

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Year of graduation: 2024



Abstract:

Age-related macular degeneration (AMD) is the third most common visual impairment globally. The disease is hallmarked by increased expression of reactive oxygen species (ROS), chronic inflammatory immune signaling, cellular and tissue damage, and eventual blindness. There is no cure for AMD and treatment options are limited. Often, the oxidative stress from inflammation and ROS is left untreated, further promoting disease progression. To provide more complete treatment of AMD, the application of a novel anti-inflammatory heme-bound human serum albumin (heme-albumin) protein complex delivered by ROS scavenging polydopamine (PDA) nanoparticles (NPs) for sustained treatment of AMD was investigated. When exposed to retinal pigment epithelial cells, heme-albumin will induce expression of the enzyme, heme oxygenase 1 (HO-1), that provides anti-inflammatory protection through the generation of carbon monoxide and biliverdin during heme catabolism. The physical and in vitro properties of heme-albumin and heme-albumin loaded PDA NPs were explored. Results show that the novel protein complex has negligible cytotoxicity to retinal pigment epithelial cells (ARPE-19) and is capable of reducing oxidative stress induced by both lipopolysaccharide and hydrogel peroxide exposure. Additionally, at 500 $\mu\text{g}/\text{mL}$, heme-albumin induces a statistically significant difference in HO-1 expression. When incorporated into PDA NPs, heme-albumin was sustainably released for up to 6 months, showing faster release at higher oxidative stress levels. Through its ability to react with ROS, heme-albumin loaded PDA NPs showed further reduction of oxidative stress. Altogether, we demonstrate that heme-albumin loaded PDA NPs reduces oxidative stress in vitro and can potentially provide sustained therapeutic delivery for AMD treatment.



B.1 Tuning aminosilica catalysts for the aldol condensation reaction to produce bio-derived surfactants

Presenter: Hannah Pineault

Advisor: Dr. Nicholas Brunelli

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Year of graduation: 2025



Abstract:

Surfactants are a key ingredient in everyday products like soap, detergent and coatings. Oleo-furan sulfonates (OFSs) are a new type of surfactant that are bio-derived and highly tunable compared to their conventional petroleum-derived counterparts. A potential synthesis route for OFSs is the aldol condensation reaction between furfural and long-chain linear ketones. This route reduces the steps in the synthesis and has the potential to be low cost. A key challenge for the aldol reaction is the selectivity, regarding both chemoselectivity and regioselectivity. Aminosilica catalysts are highly active for the aldol condensation reaction because of cooperative acid-base interactions on the catalyst surface. The goal of this work is to tune the selectivity of amine-functionalized negligible micropore (NMP) SBA-15 for the linear aldol condensation product to produce OFSs. Different amine types (primary and secondary) and the reaction temperature will be investigated.

The completed synthesis and characterization of amine-grafted NMP SBA-15 confirms its mesoporous structure and the presence of catalytic sites. Preliminary kinetic tests of both materials confirm that they are catalytically active for the aldol reaction. Future work will focus on tuning the selectivity of the catalysts. More specifically, a reaction with a symmetric ketone will be used to study the chemoselectivity between the addition and condensation product. Likewise, an unsymmetric ketone will be used to determine the regioselectivity between the linear and branched products. Overall, tuning furfural aldol chemistry for the linear condensation product will enable feasible synthesis of bio-mass derived surfactants.

B.2 Quantifying the effect of surface density of aminosilanes on the fraction of active sites in SBA-15 for the Aldol condensation

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Year of graduation: 2023



Abstract:

Cooperative interactions have been found to accelerate a range of chemical reactions, including the aldol reaction and condensation, Knoevenagel condensation, and the nitroaldol reaction and condensation. The cooperative interactions can be designed into heterogeneous catalytic materials such as mesoporous silica functionalized with an aminosilane. SBA-15 is a mesoporous silica that has attracted attention because of its high thermal stability and large surface area, and has been utilized extensively for many catalytic reactions. Additionally, the catalytic activity is affected by the structure and the density of the amine on the surface. SBA-15 has been reported to possess both mesopores and micropores, but it is not clear if the catalytic activity is different for aminosilanes grafted in mesopores versus micropores. Our group has previously found out that by limiting the micropores can increase the catalytic activity on the SBA-15. In this work, we will test the hypothesis that all amine catalytic sites are catalytically active. The functional relations between surface density with the number of active catalytic sites will be better understood through the site quantification experiment.



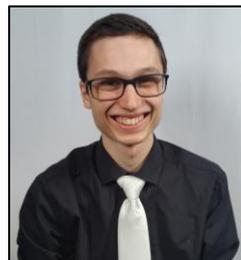
B.3 Electrocatalytic synthesis of ammonia on composite bimetallic nitride-perovskite oxide SOEC cathode

Presenter: Matthew Ferree

Advisor: Dr. Umit S. Ozkan

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Year of graduation: 2024



Abstract:

In the past century, the human population has become increasingly dependent on commercial NH_3 production to grow food, but the technology has evolved very little to keep up with the accelerating demand. In the conventional Haber-Bosch process, N_2 and H_2 are reacted at high temperatures and pressures, but the H_2 production and pressurization steps can be bypassed by using N_2 and H_2O in a solid-oxide electrolysis cell (SOEC). Perovskite oxides are known to be active cathode materials for high-temperature electrolysis of H_2O , but certain transition metal nitrides may be more capable of activating N_2 .

In this study, a composite SOEC cathode of the perovskite ($\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.95}\text{Fe}_{0.8}\text{O}_3$ (LSCF) and the nitride $\text{Co}_3\text{Mo}_3\text{N}$ was fabricated, and its activity for NRR was studied. During NRR, 3% $\text{H}_2\text{O}/\text{N}_2$ was supplied to the cathode at 500–600°C with applied current densities of 0–2 mA/cm^2 . The composite cathode performed significantly better than the pure perovskite cathode or pure $\text{Co}_3\text{Mo}_3\text{N}$ cathode, indicating a synergistic relationship between the two materials. These results imply that $\text{Co}_3\text{Mo}_3\text{N}$ increases the rate of nitrogen activation, while the ionic/electronic conduction properties of LSCF improve the overall cell performance.

$\text{Co}_3\text{Mo}_3\text{N}$ was characterized by in-situ XRD, NAP-XPS, XANES, DRIFTS, and temperature-programmed experiments to study the mobility of lattice nitrogen, stability under humid conditions, and adsorption behavior.

Few non-noble metal materials have been identified as effective electrochemical NRR catalysts for the high-temperature range. The activity of $\text{Co}_3\text{Mo}_3\text{N}$ and its compatibility with proven perovskite catalysts allow for this unique composite cathode approach to high temperature NH_3 production.



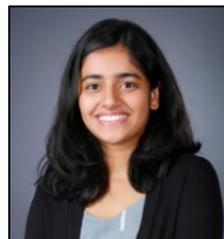
B.4 Tunable palladium catalyst using swellable organically modified silica as a scaffold for aqueous phase phenol hydrogenation

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Advisor: Dr. Umit S. Ozkan

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Year of graduation: 2025



Abstract:

Limited availability and environmental impacts of fossil sources have created a need for development of sustainable technologies using renewable feedstocks for fulfilling the ever-growing demand for energy and chemicals. Manufacturing of indispensable commodities like nylon and ester requires cyclohexanone and cyclohexanol as starting materials. While conventionally these chemicals are produced from fossil-derived crude oil, we are focusing on the selective production of cyclohexanone and cyclohexanol using bio-derived feedstock. We have developed a palladium catalyst using a novel animated organic-inorganic hybrid support- 'Swellable organically modified silica (SOMS)' for aqueous phase hydrogenation of phenol to cyclohexanone and cyclohexanol. SOMS's selective affinity towards organics and its ability to swell in the presence of organics impart SOMS, high adsorption capacity which enhances the local concentration of the reactant near the active sites, hence, promoting the reaction kinetics. SOMS being hydrophobic preserves the mechanical integrity of the catalyst during aqueous phase reaction and protects the active metal sites, unlike conventional supports like Al_2O_3 . SOMS is synthesized using sol gel method from organically modified precursor, followed by capping of the hydrophilic Si-OH groups. The synthesis procedure of SOMS was varied to modify its surface hydrophobicity. Activity experiments showed the dependence of cyclohexanol and cyclohexanone on the surface hydrophobicity of SOMS. Structural changes and the resulting effects on metal dispersion, caused by the modification in the synthesis procedure were analyzed by different characterization techniques. Thus, this work provides a unique and facile approach of synthesizing a tunable and selective catalyst for phenol hydrogenation, using SOMS.



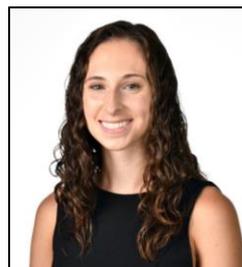
B.5 Quantifying active catalytic sites in Lewis acidic zeolite Sn-Beta

Presenter: Leah Ford

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Year of graduation: 2024



Abstract:

Sn-Beta is a promising catalyst for numerous reactions involved in biomass upgrading and fine chemical production. Interestingly, Sn-Beta is proposed to have two distinct catalytic sites: open and closed sites. The quantification of these different catalytic sites is important for understanding structure-function relationships in Sn-Beta materials. One kind of site quantification technique that is of particular interest is poisoning experiments, in which a Lewis base is added to deactivate a certain fraction of Sn metal sites before catalytic testing for a given reaction. Here, four poisons – triethylamine, pyridine, 2,6-lutidine, and trimethylphosphine oxide (TMPO) – are tested in site quantification poisoning experiments using epichlorohydrin ring opening by methanol. As demonstrated experimentally, the results are robust with little to no effect of diffusion limitations on the data. Triethylamine and pyridine are able to distinguish catalytic sites with different levels of activity by preferentially deactivating sites with higher activity, evidenced by multi-slope decreases in turnover frequency. 2,6-lutidine and TMPO, however, are unable to make this distinction, likely because of steric hindrance and solvent effects, respectively. Poisoning experiments conducted on different Sn-Beta materials provide evidence that the fraction of highly active sites (increases/decreases) with increasing crystallization time, likely accounting for the (increase/decrease) in activity. The identification of appropriate poisons will contribute to the establishment of robust procedures for Sn-Beta site quantification, which in turn will enable the determination of effective Sn-Beta synthesis parameters.



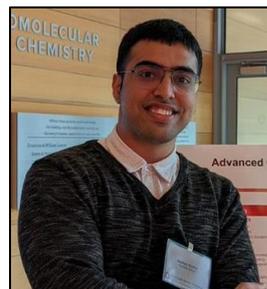
C.1 Constrained robust Bayesian optimization of expensive black-box functions under uncertainty

Presenter: Akshay Kudva

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Year of graduation: 2024



Abstract:

Modern engineering problems requires its systems to not just behave optimally but also in a robust manner. The notion of robustness requires the system to take into account safety, efficiency, flexibility etc in the presence of adversarial variables that can perturb the system into a worst-case scenario. Many such engineering systems are often simulated by complex models that allows practitioners to evaluate the performance of these engineering systems. In certain situations, one may develop equation oriented (EO) or “white-box” models from which the first and/or second derivative can be exploited for optimization. However, often times, these complex models or simulators are expensive to evaluate, non-smooth and derivatives may be unavailable which makes these problems challenging to optimize. Typically, such problems are optimized using derivative free optimization (DFO) or zero order methods like Bayesian optimization (BO) which queries function sequentially. An adversarially robust optimizer must select a “robust design” such that its corresponding worst-case scenario is always less than the worst-case scenario of an alternate design (minimax settings). The optimization problem becomes even more challenging in the presence of constraints with unknown structure. In this work, we present a novel algorithm which is one of the first to address constrained robust optimization of noisy and expensive-to-evaluate functions under BO settings. The effectiveness of the proposed framework is demonstrated by implementation on a benchmark problem and a high-fidelity bio-reactor simulator.

C.2 A new optimization-based framework for learning efficient multivariate quadrature rules

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Advisor: Dr. Joel Paulson

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Year of graduation: 2026



Abstract:

Integration is a fundamental operator in modeling engineering systems and is the foundation of all modern statistics. Any time when random variable is involved in the systems, we must integrate over its density function. However, often times there are cases where the function doesn't have an antiderivative or it's too complex to be integrated analytically in multiple dimensions. Numerical integration are algorithms that approximate the numerical value of a definite integral. The most common method is Monte Carlo due to its generality, but the generality comes at the cost of slow convergence rate which limits its applicability to expensive computer simulators. Many emerging models of next-generation systems are becoming very expensive due to the multi-scale nature of many important problems (e.g., climate change). A promising alternative is Gaussian quadrature, which is a well-established method that reduce the cost of MC. Gauss quadrature specifically selects nodes and weights in an ordered/non-random fashion; however, it is non-trivial to extend this method to higher dimensions and non-polynomial functions. We propose a framework that can extend Gaussian quadrature to higher dimensions and more general types of functions. The main idea is to formulate the search for a quadrature rule as an optimization problem. Although this problem is difficult to solve exactly, we propose a new machine learning-based approach that can approximately solve this problem efficiently. We demonstrate the effectiveness of the proposed framework compared to competing alternatives on several problems related to uncertainty quantification including simulation of quantum mechanical systems and stochastic decision-making problems.

C.3 Using bioinformatics and computational protein design to increase selectivity for butanol production from engineered *Clostridium tyrobutyricum*

Presenter: Curtis Moore

Advisor: Dr. Shang-Tian Yang

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Year of graduation: 2025



Abstract:

Butanol derived from acetone-butanol-ethanol (ABE) fermentation (i.e., biobutanol) has potential to replace gasoline as fuel for automobiles powered by internal combustion engines. We seek to greatly improve the butanol selectivity and productivity of the biobutanol fermentation by engineering the bacteria *C. tyrobutyricum* with a heterologous gene that encodes for an aldehyde-alcohol dehydrogenase (AAD) enzyme. The discovery of this heterologous gene will be performed by mining protein sequence databases for similar enzymes, a procedure typically referred to as bioprospecting. AlphaFold2 will be used to generate protein structures from the mined sequences. Ligand Docking in Rosetta will then be performed using the generated models and the reaction intermediate of the enzyme's respective reaction. The ligand/protein interface score from these docking studies will be used to evaluate each protein's ability for performing their respective reaction. The most promising protein sequences will then be expressed in *E. coli*, and their enzymatic activity will be determined via assay. We will then use computational protein design to improve the selectivity of the enzymes displaying the highest activity. For this procedure Rosetta enzyme design will be used to mutate residues in the active site of these enzymes to enhance enzyme selectivity. Our goal is to discover novel enzymes capable of performing our reaction of interest using in-silico enzyme screening, then design these enzymes for higher selectivity towards our product of choice, butanol, using computational enzyme design.



D.1 Magnetic field induced concentration gradient of SPIONs studied by in-situ small angle X-ray scattering

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Year of graduation: 2024



Abstract:

With the rapid development of nano-material synthesis technologies, a series of superparamagnetic iron oxide nanoparticles (SPIONs) have been produced with special physical properties, such as high surface to volume ratio, biocompatibility and superparamagnetism. Nevertheless, due to the nanometric size of SPIONs, the magnetically driven isolation methods to separate those particles from the media is difficult, considering the fact that the Brownian motion and viscous drag will hinder the magnetic motion of the particles.

In our previous work, we reported the ability to recover 5, 15 and 30 nm particles by applying external magnetic fields and gradients. Our experimental data suggest that the particles suspension have concentration gradient due to fluid diffusion or possible dipole-dipole interactions. However, the nano-structural changes of particles with applied magnetic field and the mechanisms behind the separation processes are not fully understood.

In order to gain insight into the separation mechanisms, we conducted the *in-situ* study of SPIONs magnetic separation using Small Angle X-ray Scattering (SAXS), which is an ideal and powerful characterization tool that can provide precise structural information of the particle agglomeration. The *in-situ* analysis tracked the evolution of particles diameter, volume fractions as well as particle number density. Two special magnetic separation sorters were used, allowing the X-ray pass through the tubing that holding the particles while being magnetized by the external field. Multiple variables and parameters are studied, including operation time, the magnetic field gradient and intensities.



E.1 Elucidating the correlation between ion transport and structural heterogeneity in triazole-based polymerized ionic liquids

Presenter: Javad Jeddi

Advisor: Dr. Joshua Sangoro

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Year of graduation: 2024



Abstract:

The relationship between chemical structure, nanoscale organization, and ion transport in 1,2,3-triazole-based polymerized ionic liquids (PILs) was investigated by wide-angle X-ray scattering (WAXS) and broadband dielectric spectroscopy (BDS). The DC ionic conductivity of PILs was correlated with the glass temperature transition (T_g) in which low T_g PIL exhibited higher ionic conductivity. Analyzing the WAXS and BDS results indicated that mobile ion type and chemical structure of the pendant groups both controlled structural heterogeneity and ion conduction of the PILs below T_g . The normalized heterogeneity length extracted from the WAXS data was used to correlate the structural heterogeneity and ion conduction activation energy. For the polycation samples, the large TFSI⁻ mobile ion results in a higher packed structure than the small Cl⁻ anion while in the polyanion samples inverse trend was observed. The estimation of the activation energies of the DC conductivity below T_g measured by BDS is quantitatively correlated to the structural heterogeneity obtained from nanostructure analysis using WAXS. This suggests that increasing the spatial heterogeneity of the PILs leads to the reduction in activation energy barriers of long-range ion motions. These results highlight the role of spatial heterogeneity in designing efficient polymerized ionic liquids.

E.2 Polyamidine-based membranes for highly selective CO₂/N₂ separation

Presenter: Jingying Hu

Advisor: Dr. W. S. Winston Ho

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Year of graduation: 2023



Abstract:

Amidines are perceived as better alternatives for amines in the facilitated transport membranes for having faster CO₂ reaction kinetics. The synthesis of poly(ethylene formamidine) (PEF) was carried out via the polycondensation of ethylenediamine and triethyl orthoformate catalyzed by acetic acid. The synthesized PEF possessed the highest amidine functional group density owing to the case using the shortest diamine, ethylenediamine. Moreover, compared with small amidine-containing molecules, PEF exhibited a much higher boiling point, which practically eliminates the possibility of the leaching out of amidine moieties. For membrane synthesis, PEF (10 kDa MW) was blended with polyvinylalcohol (PVA, 1.1 MDa MW) and then coated onto nanoporous polyethersulfone (PES) substrates to form a composite membrane with 170-nm thick selective layer. Increasing the PEF content from 36 wt.% to 66 wt.% in these membranes led to a substantial increase in membrane performance, especially for CO₂ permeance. Further increasing the PEF content to 83 wt.% still enhanced the CO₂ permeance but resulted in a moderate drop in CO₂/N₂ selectivity. Under an extremely high PEF content of 90 wt.%, the membrane showed a low CO₂ permeance of 1019 GPU but a high CO₂/N₂ selectivity of 236, indicating severe pore penetration. Overall, the membrane containing 83 wt.% PEF exhibited the best performance of 2807 GPU CO₂ permeance and 72 CO₂/N₂ selectivity.



E.3 Ion dynamics in single-ion and salt-doped polymer electrolytes via coarse-grained simulations

Presenter: Mengdi Fan

Advisor: Dr. Lisa Hall

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Year of graduation: 2023



Abstract:

Salt-doped block copolymers (BCP) are widely explored as solid-state electrolytes for their ability to combine ion conduction and mechanical robustness. However, besides the relatively low ion conduction compared to liquid electrolytes, the salt-doped BCPs also have lower lithium ion transference number t_+ which represents the fractional contribution of cations to overall conductivity. As cations and anions are freely moving in salt-doped BCPs, ions may form natural ion pairs or aggregations and can not efficiently contribute to conduction. On the other hand, the single-ion structure which tethers anions to the polymer backbone can improve the lithium ion transference number by limiting the motion of anions to the immobile polymer backbone, though it may suffer from lower ion conduction due to the slower overall dynamics. To compare the difference between single-ion and salt-doped systems in a controlled way, we use coarse-grained molecular dynamics simulations to study the two systems with the bonds between anions and monomers as the only difference between the two types of systems. We studied the effects of ion concentration and polymer dielectric constant and explored the impacts of tethering position on ion structural properties and dynamics. We find single-ion structure can facilitate cation conduction at relatively lower ion concentrations and dielectric constants.



E.4 Biomimicking liquid crystal elastomers with densely packed nanowire structures exhibit stimuli-responsive curling, locomotion, and transportation

Presenter: Robert Dupont

Advisor: Dr. Xiaoguang “William” Wang

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Year of graduation: 2024



Abstract:

Liquid crystalline materials have seen recent success in the areas of targeted drug delivery, soft robotics, sensors, actuators, and surface structures. From macroscopic design to microscopic construction, much of these successes have looked to nature for inspiration. Following suit, the presented research focuses on the macroscopic level with the creation of a liquid crystalline elastomeric film with a forest of nanowires on one side, mimicking gecko foot pads and filefish scales. These films are created using an anodized aluminum oxide template and take advantage of the inherent self-aligning properties of liquid crystals. These films exhibit macroscopic curling deformations in response to external stimuli such as heat and common solvents. As typical for liquid crystal elastomers, these macroscopic deformations are reversible and repeatable, with our films showing the same magnitude of deformation over at least 100 cycles with linear response to a change in temperature between 60 and 150°C. In addition, when the films are exposed to common solvents like toluene, the direction of their deformation depends on the phase of the solvent, with the response to solvent vapor behaving similarly to the response to temperature and the response to droplets of solvents being in the opposite direction but with the same magnitude. Finally, modifying the films through silanization and a Michael addition reaction enhances their natural, structure-based superoleophobicity allowing them to be used to transport oily chemicals underwater for use in reactions and droplet transport.

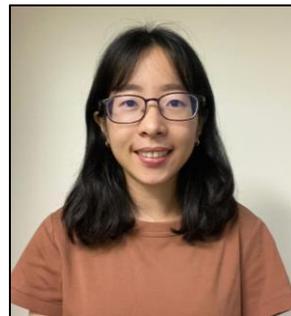
E.5 Feasibility of membrane-adsorption hybrid process for direct air capture

Presenter: Yi-Chen Huang

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Year of graduation: 2024



Abstract:

The direct CO₂ capture from ambient air could mitigate CO₂ emissions from non-stationary sources. However, the level of the atmospheric CO₂ is only about 410 ppm, which imposes challenges for DAC if a high CO₂ purity is required. Recently, amine-containing polymeric membranes with exceptional CO₂/N₂ selectivity have been developed for CO₂ capture. Nevertheless, a high degree of air compression is needed to provide the transmembrane driving force, which makes the application prohibitive. Another approach for DAC is to employ solid sorbents with high CO₂ capacity, but the limited stability of the sorbent and the high regeneration energy usually lead to a high capture cost. In this work, we propose a membrane adsorption hybrid process for DAC, where a less CO₂-selective yet robust physisorbent is used to enrich the CO₂ to 40%. This desorbed CO₂ is then further purified by a highly CO₂-selective membrane, where the higher feed CO₂ concentration relaxes the compression requirement. Then techno-economic analyses of the hybrid process are studied to evaluate the feasibility of the hybrid process for DAC.



E.6 Local analysis of ion structure and dynamics in coarse-grained simulations of block copolymer electrolytes with homopolymer additives

Presenter: Yuanhao Zhang

Advisor: Dr. Lisa Hall

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Year of graduation: 2025



Abstract:

Salt-doped block copolymers (BCP) are promising solid electrolytes because of their ability to form two distinct microphases which allow for ionic conductivity along with significant mechanical strength. Recent study has shown that the addition of relatively high molecular weight (MW) homopolymers of the same chemistry as the conductive phase will form a relatively mobile homopolymer-rich region with higher ion concentration in the center of conducting microphase, leading to a higher overall ion conductivity. We use coarse-grained molecular dynamics simulations to understand the correlation between the distribution of each component (influenced by the chain length and concentration of ions and additives) and the local motion of ions or ion conductivity. We use a simple bead-spring model with Lennard-Jones (LJ) interactions between all beads, Coulomb interactions between ions, and additional solvation interactions of the form $-1/r^4$ between ions and the beads of the conducting block. Microphase separation is driven by relatively unfavorable LJ interactions between conducting and non-conducting type beads, and the dynamics of the nonconducting beads are slowed (T_g is increased) by increasing the like-like LJ interaction strength for those beads. We analyze the distribution of ions and homopolymers with different MWs. We also calculate the local ion mobility as a function of distance across the microphase domain, showing clear differences in the dynamic behavior of ions based on their location. The local polymer relaxation time and number of ion neighbors around a given ion will also be discussed to explain the mobility distribution.



E.7 Fabrication of semi-commercial-size countercurrent spiral-wound membrane modules for CO₂ capture from flue gas

Presenter: Yutong Yang

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Year of graduation: 2023



Abstract:

Despite the tremendous progress made in the synthesis of high-performance polymeric membranes, only a few membrane technologies were advanced to the bench-scale study. The module fabrication is a nontrivial method to realize the commercialization of gas separation membranes for post-combustion carbon capture, but is rarely demonstrated. An $\varnothing 8''$ semi-commercial-size countercurrent sweep spiral-wound (SW) membrane module was successfully fabricated. This module was intended for the retentate recycle operation as an internal sweep. The element contained 41 membrane leaves, each with a width of 20" and a length of 36", resulting in a membrane area of 35 m². To ensure an even distribution of the sweep flow on the permeate side and avoid "dead zones" near the edges of the membrane leaf, a new epoxy glue dot line with a strategically designed pattern was developed to decrease the pressure drop and have a countercurrent flow configuration. A pair of prototype anti-telescoping devices (ATD) was glued to the two ends of the element to stop the bypass of feed gas and hence enhance the CO₂ transport in the element. A thin layer of fiber reinforcement plastic (FRP) was wrapped to increase the packing density. The SW membrane modules demonstrated essentially no leakage. The pressure drop was 0.9 psi/m at the designed flow rate of 170 sccm/m², corresponding to the retentate recycle at 15% of the total retentate flow rate, which met the requirement of ≤ 1.5 psi/m for the pressure drop of the SW membrane module.

E.8 Microstructure engineered topological defects: Enabling new applications of liquid crystals

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Year of graduation: 2024



Abstract:

Liquid crystals (LCs) are a thermodynamically stable phase of condensed matter that combines the long-range orientational order associated with crystalline solids with the fluidity of isotropic liquids. The mobility of LC mesogens, in conjunction with their long-range order, allows for the rapid reorganization and communication of information across the LC bulk. This unique property of LCs makes them respond relatively quickly to external stimuli such as electrical and magnetic fields, pressure, light, temperature, and chemical and biological species. In the past, extensive studies have been conducted to characterize electrical and magnetic fields' effect on the orientation of LCs, which led to the development of the liquid crystal display (LCD). Also, several fundamental studies have been conducted to understand the interaction of LC mesogens with different chemically functionalized surfaces leading to the development of LC-based chemical and biological sensors. However, there have been very limited studies investigating the response of LCs to physical stimuli such as mechanical shear. In this work, we investigate the response of microstructure confined LCs to mechanical shear and leverage the unique behavior of this system to develop new design principles for the simple, sensitive, and real-time visualization of fluid flow fields in microfluidic systems. In addition, we also show that the shear-induced reorientation and long-range elastic fields associated with microstructure confined LCs can be exploited to control, assemble, and transport colloidal particles.

E.9 Selective H₂S/CO₂ separation using sterically hindered amine membranes

Presenter: Shraavya Rao

Advisor: Dr. W.S. Winston Ho

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Year of graduation: 2023



Abstract:

H₂S, an extremely toxic and corrosive gas, is a common contaminant in fuel gas mixtures such as syngas and natural gas. The selective removal of H₂S from such CO₂-containing fuel gases is important for enabling their industrial processing. This work describes the development of amine-based facilitated transport membranes (FTMs) with high H₂S/CO₂ selectivity at elevated temperatures (>100°C).

A series of amine carriers with varying structure was used to synthesize FTMs and their H₂S/CO₂ transport performances were investigated. Sterically hindered amines showed enhanced H₂S/CO₂ separation performance, with the H₂S/CO₂ selectivity rising from 4 to nearly 20 as the amine hindrance was increased. The best performance was obtained using a severely hindered di-*tert*-butylamine carrier, which showed a high H₂S/CO₂ selectivity of 19.6 and an H₂S permeance of 560 GPU. These results are supported by density functional theory calculations, which showed that amine hindrance can restrict the amine-CO₂ reaction without affecting the amine-H₂S reaction. Finally, the carrier saturation behavior of the di-*tert*-butylamine carrier was investigated at H₂S concentrations of 0.5—30%, obtaining H₂S/CO₂ selectivities of 25 — 9 and H₂S permeances of 760—220 GPU. Overall, the newly devised membranes show good potential for syngas desulfurization, and the learnings offer some insight into the mechanisms of acid gas transport in amine membranes.



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