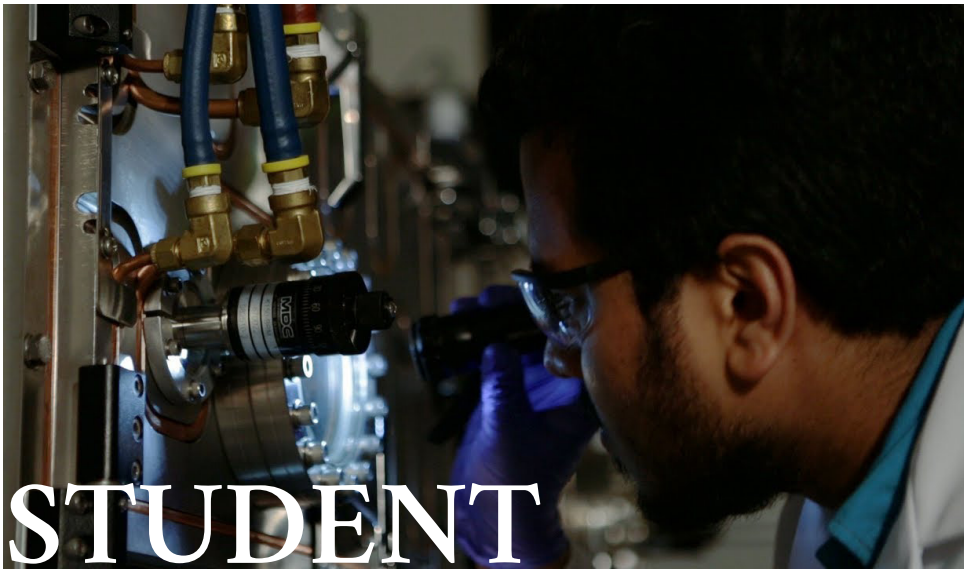
RESEARCH FIRST LOOK

A glimpse into the latest graduate and postdoctoral energy research at the University of Houston

UH Energy
UNIVERSITY OF HOUSTON



STUDENT RESEARCH AT UH

Undergraduate Research

The Office of Undergraduate Research and Major Awards provides support, resources, and research opportunities for undergraduate students through faculty-mentored research programs. Research enables you to work one-on-one in collaboration with a faculty mentor, and to contribute to original scholarship at the undergraduate level. By conducting research, undergraduates have the opportunity to hone communication skills, collaboration, creativity and critical thinking. Students also hone their leadership skills and professional development to better prepare for life upon graduation.

Graduate Research

The UH Graduate School cultivates and supports academic excellence in graduate and professional education. A Carnegie-designated Tier One Research University, UH offers master's degrees in 133 fields and doctoral degrees in 62 fields. With more than $250 million in research expenditures in fiscal year 2022, UH offers more than 6,000 graduate students rich opportunities to research under top scholars, who are invested in basic research and translating that research into real-life applications and technologies.

Division of Research
UNIVERSITY OF HOUSTON

Graduate School
Office of the Provost

UH Energy
UNIVERSITY OF HOUSTON

ENERGY RESEARCH DAY

AUGUST 30 | 4 -8 PM | STUDENT CENTER SOUTH MULTIPURPOSE ROOM

AGENDA

4:00 PM — **WELCOME AND OPENING REMARKS**

Dr. Ramanan Krishnamoorti, Vice President of Energy & Innovation, ***University of Houston***
Dr. Claudia Neuhauser, Vice President of Research, ***University of Houston***
Dr. Sarah Larsen, Dean of Graduate School, ***University of Houston***

4:15 PM — **KEYNOTE SPEAKER**

Dr. Harriet Kung - Deputy Director for Science Programs
Office of Science, U.S. Department of Energy

4:45 PM — **Q&A FROM AUDIENCE**

5:00 PM — **INTRODUCTION OF PANEL: THE ROLE OF RESEARCH IN THE ENERGY INDUSTRY**

Dr. Ramanan Krishnamoorti, Vice President of Energy & Innovation, ***University of Houston***

5:10 PM — **PANELIST INTRODUCTIONS & OPENING REMARKS**

Cynthia Ginestra, ***Shell***
Juliana Garazier, ***Greentown Labs***
Sindhu Balan, ***Chevron***
Sujatha Kumar, ***Dsider***

5:40 PM — **MODERATED PANEL DISCUSSION**

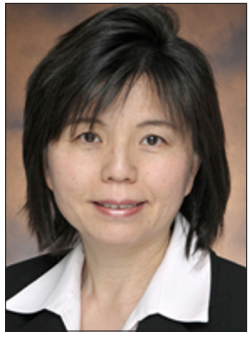
5:50 PM — **Q&A FROM AUDIENCE AND CLOSING REMARKS**

6:00 PM — **STUDENT POSTER SHOWCASE AND NETWORKING UNTIL 8:00 PM**

Dr. Harriet Kung (KEYNOTE SPEAKER)

Deputy Director for Science Programs, Office of Science

U.S. Department of Energy



Dr. Harriet Kung is the Deputy Director for Science Programs in the Office of Science at the U.S. Department of Energy. As Deputy Director for Science Programs, Dr. Kung is the senior career official providing scientific and management direction and oversight for the Office of Science research programs, including Advanced Scientific Computing Research, Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, High Energy Physics, and Nuclear Physics, as well as other supporting functions and offices.

Prior to serving in this position, Dr. Kung served in various leadership roles in Basic Energy Sciences, the largest program in Office of Science, from 2002 - 2020. Before joining DOE in 2002, Dr. Kung was a technical staff member and a project leader at Los Alamos National Laboratory. Her research focused primarily on nanoscale materials and high temperature superconductivity.

With over 20 years of service in the Department of Energy, Dr. Kung led and cultivated one of the Nation's premier research programs in the physical sciences. During her tenure, she developed a new basic research paradigm, fostering a team-science approach to advance DOE's science and energy missions by spearheading a decade-long strategic planning initiative to assure timely, science-based solutions.

She also positioned the Office of Science as a National Quantum Initiative leader by establishing strategies to capitalize on strong synergies between disciplines, such as physics, biology, materials, computation, and engineering, as well as its world-leading scientific user facilities. She has chaired and co-chaired high-level interagency working groups to develop and implement national science priorities.

Dr. Kung received her M.S. and Ph.D. degrees from Cornell University. She is the recipient of numerous awards including the Presidential Meritorious Executive Rank Award in 2009 and the Distinguished Executive Rank Award in 2022.

Dr. Sindhu Balan

Investment Principal

Chevron Technology Ventures

Sindhu Balan is an Investment Principal in Chevron Technology Ventures (CTV). CTV addresses Chevron's business needs through the identification and integration of innovative externally developed technologies that strengthen Chevron's business now and in the future. Sindhu joined Chevron in 2009 as a business analyst and has held several positions in Strategy and Planning, Upstream, Downstream, Technology Ventures and the Technical Center. Sindhu's work experience external to Chevron spans IP, investments, and R&D for the pharma industry. Sindhu holds a bachelor's degree in pharmacy and a master's degree in technology (Bioprocessing / Downstream) from the University of Mumbai (India), a doctoral degree in Biochemistry & Biophysics and an MBA from the University of Houston.

Juliana Garaizar

Chief Development and Investment Officer

Greentown Labs

Juliana is the Chief Development and Investment Officer at Greentown Labs. A Board Member of the Angel Capital Association, Juliana is a Lead Investor of the Portfolia Rising America Fund that invests in BIPOC and LGTBQ founders, as well as the Portfolia Consumer and Rising Tide Funds. She is also an Advisory Board Member of the University of Houston Cougar Venture Fund, the Houston Diversity Fund, the Investors of Color network and Impulse4women. A Kauffman Fellow experienced in Bridging the Gender Gap in investing, she is part of the City of Houston's Women Commission. Juliana was the Texas Medical Center Venture Fund Director and the Managing Director of the Houston Angel Network. She was the Manager of the French Riviera's Sophia Business Angels network and Antipolis Innovation Campus and Project Manager of several International Projects funded by the European Commission. Previously, Juliana worked for five years in Singapore: first as an International Trade Consultant for the Trade Commission of Spain in a broad range of industry sectors and then as a Project Manager for the Asia Technology Office of Citigroup, leading projects at the international level. Juliana obtained an MBA at the London Business School and Haas School of Business in Berkeley, specializing in Entrepreneurship.

2023 ENERGY RESEARCH DAY SPEAKERS

Dr. Cynthia Ginestra

Sustainable Products Market Development Manager

Shell

Dr. Cynthia Ginestra, a clean energy champion at Shell since 2012, has driven innovation across various roles, from sustainable aviation fuels to electric mobility. Leading technology teams, she bridges lab-to-market for cleantech and empowers future innovators. Cynthia holds a Ph.D. in Materials Science and Engineering, an MS in Management Science from Stanford, and a BS in Physics from UT Austin. She excels at nurturing innovation inside and outside of Shell's tech teams. Cynthia is a Houston native and first-generation French American. Recently returned from two years working in The Netherlands, Cynthia now lives in Katy, Texas, with her husband and their three Energizer-bunny kids.

Sujatha Kumar

Founder and CEO

Dsider

Sujatha is an entrepreneur who has successfully led multiple technology companies throughout her career. She has also held senior executive positions at Delphi Automotive, Orano, and Honeywell. With considerable experience in both operations and digital domains, she possesses a passion for introducing innovative products and concepts to organizations. In 2014, she founded Ayatis, her digital consulting company, aimed at assisting Energy and Petrochemical companies in their operational and digital transformation journeys, with a focus on decision intelligence technologies. Currently, Sujatha holds the role of founder and CEO at Dsider, an integrated Net Zero planning software platform designed to help companies navigate sustainably to Net Zero through informed decisions. In addition to her responsibilities at Dsider, Sujatha serves as an advisor at Knightsgate Ventures and collaborates with various startups. She also contributes her expertise as an advisor and board member to both public companies and startups.

CULLEN COLLEGE OF ENGINEERING

MECHANICAL ENGINEERING

Physics-based AI platform on thin film evaporation in hierarchical structures

Research Themes

• Foster a physics-informed ML platform on thin film evaporation in hierarchical structures and complement this platform through new knowledge on small-scale phase- change phenomena.

• Capture an unsolved relationship between heat flux vs geometrical and physical variables via data science.

• To develop novel hierarchical structures with exceptional heat flux performance.

Issues

• Proving the generality of the AI model.

• Practicality of the developed structure.

Recent Accomplishments

• We used Physics-Informed Neural Network (PINN), to train and validate an AI model. The AI model shows a good performance in prediction of heat flux as a function of independent variables.

• We developed a structure using Genetic Algorithm.

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ME

Robotic Fish enabled Co_2 Monitoring

Research Themes

- Underwater bio-inspired robotics
- CO_2 monitoring and detection of leakage source using swarm of robotic fish

Issues

- Bio-inspired improved propulsion efficiency
- Modeling and control of underactuated system
- 3D Maneuvering
- Swarming control in the limitation of low-bandwidth communication
- Low resolution of localization

Recent Accomplishments

- Depth Control Device and model predictive depth control design and implementation
- Design of 3D robotic fish and experimental testing in the swimming pool
- AI-enhanced swarming control

Umar Masood

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ME

Monitoring of State of Charge of Li-Ion Battery

Research Themes

• Effective state of charge (SOC) monitoring methods for Li-ion batteries are critical toensure that they operate in the healthy status.

• Utilizing the ultrasonic method to assess the SOC of the organic Li-ion coin cell by themachine learning/deep learning model.

Issues

• Recent research based on ultrasonic method and machine learning/deep learning has focused on the Li-ion pouch cell. The research on the SOC estimation of the organiccoin cell by the ultrasonic method is limited.

Recent Accomplishments

• Developed a deep-learning-based method for the SOC prediction of the organic coin cell.

• The preliminary results show that the machine learning/deep learning model canachieve a relatively good estimation on the SOC prediction of the organic coin cell.

• When the charging/discharging current increases, the SOC estimation performance can be improved.

Jian Chen

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ME

Cable-Driven Parallel Robot Manipulator

Research Themes

• Develop an easily adaptable automated system capable of positioning a waterproof transmitter coil within an underwater workspace

• Implement multiple closed loop controllers using encoders and load cells to increase position accuracy of the end effector

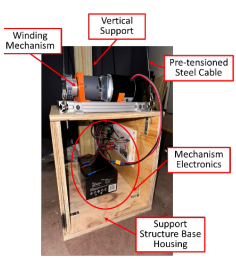
• System must maintain a low level of interference with the Magnetic Induction experiments that are being conducted

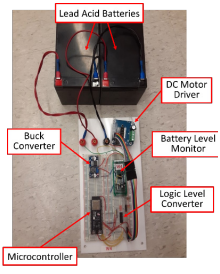
Issues

• Commercially available rigid-linked automated solutions are not practical due to the nature of the workspace. An unknown amount of error creep is present which does not allow for extended runs of the system without the need to recalibrate. There is a large delay between the user input and the movement of the robotic manipulator leading to large amounts of dead time over the course of the data gathering experiments.

Recent Accomplishments

• The current implementation can successfully move a 15 lbs. end effector within a 16' x 32' x 5' workspace up to a total of 4 times before becoming inaccurate. Before error creep is present, the positional error was measured to be less than 10 cm. A custom MATLAB App has been created in order to simplify the wireless communication to and from the four individual reeling mechanisms being used.





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ME

Hydrogen Storage Through Confined Hydrogen Hydrate

Research Themes

• Form hydrogen hydrate at a moderate pressure and temperature within the range of the Department of Energy's (DOE) target.

• Develop a more effective technique to resolve the kinetic issues involved in the charging and discharging process of hydrate formation.

Issues

• The material platform is a modified zeolite with rationally tuned pores and modified surface chemistry that stores hydrogen gas in the form of hydrogen hydrates with fast charging process at low pressure.

• We boosted the storage capacity of hydrates by 200 times compare to bulk water/THF.

• We have enhanced the discharging rates at room temperature, eliminating the need for high temperatures.

Recent Accomplishments

• Increase storage capacity of designed material to meet DOE targets.

• Develop a material to maintain hydrate stability at atmospheric pressure and room temperature.

Rojan Firuznia

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ME

Icephobic Coatings: Passive Ice Protection for Energy Applications

Research Themes

- Surface Chemistry
- Mechanics of Materials
- Polymer Science
- Heat Transfer

Issues

- Long-term durability of the state-of-the-art coatings not addressed
- Low ice adhesion performance in real-world applications
- Lack of comprehensive model for ice adhesion strength

Recent Accomplishments

- Developed durable icephobic coatings known as “Fracture-controlled surfaces”.
- Passed various tests in the lab. and third-party industrial partners in aerospace.
- Developed a comprehensive and predictive model for ice adhesion strength on a wide range of materials.

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ME

Practical Implementation of Organic Electrochemical Transitor (OECTs) for Subsea Detection

Research Themes

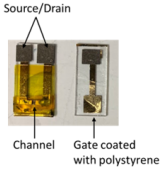
• Organic Electrochemical Transistor sensors have great potential in various applications due to their low-voltage operation, large signal amplification, enhanced sensing capabilities and sensitivity.
• We focus on using OECT sensors to detect different chemicals or contaminants by reading the source-drain current. The ultimate goal is to integrate the sensor with the marine robot to form an array of sensors capable of detecting multiple chemicals and/or localizing the source of a leak in the subsea environment.

Issues

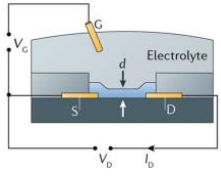
• In sensor there is a reusability issue while testing i.e; the gate, drain and source must be washed in ethanol and dried before testing in different solution

Recent Accomplishments

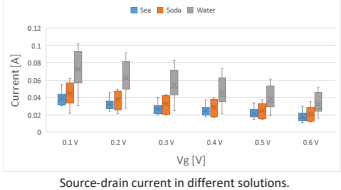
• Developed an OECT sensor consists of gate electrode adjacent to an organic semiconductor source-drain channel (PEDOT:PSS (poly(3,4-ethylenedioxythiophene) polystyrene sulfonate). The gate electrode and source-drain channel are connected via an electrolyte solution containing mobile ions. Several tests have been conducted by changing gate voltage from 0.1v to 0.6v where drain & source voltage is kept constant at 0.6v and recorded the different solutions.



OECT sensor



Sensing diagram



Source-drain current in different solutions.

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ME

CULLEN COLLEGE OF ENGINEERING

CHEMICAL ENGINEERING

Spatial and Multiplicity Trends for Tri-Reforming of Methane

Research Themes

• Utilizing methane oxidation to provide in situ heat for dry and steam reforming.

• Examining the existence of regions of multiple steady states for methane oxidation on a Pt/Pd monolith catalyst.

• Using spatially resolved measurements to observe the interplay between exothermic and endothermic reactions within a singular reaction system.

Issues

• Using reforming reactions to turn a flue gas stream into value added chemicals in syngas results in a delicate balance between conversion of methane while avoiding production of carbon dioxide.

• Usage of precious metal catalysts to perform methane oxidation is an expensive option.

Recent Accomplishments

• Observed distinct spatial regions of oxidation of methane followed by methane reforming.

• Found feed concentrations that result in the methane oxidation system exhibiting multiple potential steady states, with those states having the potential to coexist in separate monolith channels.

Jonathan Ratcliff

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ChBE

Dynamic Transient Micro-Kinetic Modelling Toolkit

Research Themes

• Performing microkinetic modelling to gain insight that help design better reactors.

• Exploration of dynamic catalysis operation of which has been proven to enhance production yield.

• Utilizing advance computation techniques to analyze experimental data and improve kinetic models.

Issues

• The multipurpose computational toolkit can model dynamic reaction operation.

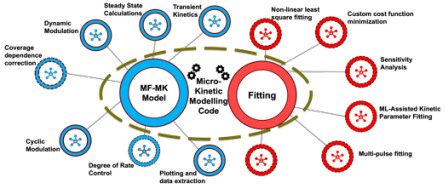
• This toolkit can analyze any reaction mechanism allowing for chemistry exploration as well as a study of potential dynamic enhancement capabilities.

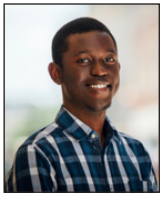
• It allows for the use of machine learning to perform improved fits that mimic experimental results.

Recent Accomplishments

• More rigorous uncertainty analysis techniques need to be implemented for fit validation.

• Implementing more robust fitting algorithms and applying fitting to dynamically obtained experimental data.





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ChBE

Electrifying the Future: CO_2 Free H_2 Production through Electric Heating

Research Themes

• Developing synthesis procedure for deposition of catalyst powder on electrically heated metallic surface.

• Achieving thermally stable coat with uniform active metal distribution on highly curved metallic structures.

• Kinetics of steam methane reforming (SMR) on coated catalysts under electric heating and optimization of hydrogen yield.

Issues

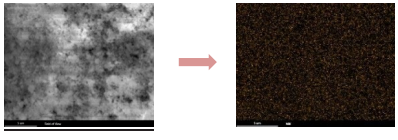
• Successfully deposited Ni-ZrO_2 catalyst on FeCrAl wires with uniform 'Ni' dispersion on coat surface by developing catalyst slurry, adjusting parameters such as pH, viscosity, ball milling time.

• Understanding kinetics of SMR on Ni-ZrO_2 powder catalyst.

Recent Accomplishments

• Expanding diversity of electrically heated coated catalysts: Improving other coated catalysts such as Ni-Al2O3 coat which exhibits 'Ni' particle agglomeration issue.

• Micro-level understanding of electrically heated catalyst for H2 production: Exploring the role of thermal electrons that origin from electric heating on reaction mechanism and catalyst performance.



SEM-EDAX analysis of Ni-ZrO_2 coat and 'Ni' dispersion on the coat

Meghana Idamakanti

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ChBE

Directed Evolution of Alkylsuccinate Biosensors Based on the ItcR Transcriptional Regulator

Research Themes

- Biological Activation of Short-chain Hydrocarbons in Anaerobic Environments
- Design and Engineering of Biosensors for Alkylsuccinate Biosynthesis

Issues

- Enzyme Specificity for Hydrocarbon Conversion
- Optimization of Biosensor Performance for Molecular Reporting

Recent Accomplishments

- Designing ItcR-Based Biosensors for Methyl-Succinate Detection
- Obtaining ItcR-based variants showing transcriptional response toward Ethyl-succinate and Methylpentyl-succinate.

Ehsan Bahrami Moghadamn

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ChBE

Tunable Functionalization and Repurposing of Polyolefin Waste to Polyurethanes

Research Themes

- Upcycling of waste plastics to durable value-added goods
- Impact of polyolefin molecular parameters in final product (polyurethanes)

Issues

- Polyolefins (POs) represent the largest contribution to plastic production, use and generated waste worldwide yet their recycling rate are low (< 9%)
- More efficient methods of recycling polyolefins have to be explored and push towards a circular economy

Recent Accomplishments

- Sustainability related internship with BASF
- The National GEM Consortium Fellowship
- UH Foundation and UH Presidential Fellowships

Ronard Herrera

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ChBE

Direct Air Capture Using Porous Metal Hydroxides

Research Themes

• Existing direct air capture (DAC) solid sorbents have high estimated sorbent costs from costly manufacturing process and limited sorbent lifetime

• Developing a novel, cost-effective and oxidation-resistant porous metal hydroxides for practical applications of DAC

Issues

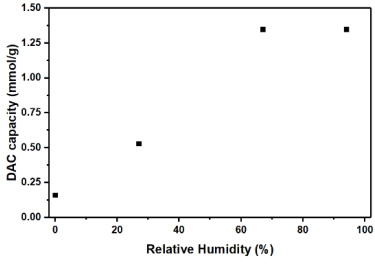
• Limited DAC capacity likely from insufficient porosity and weak CO2 binding strength

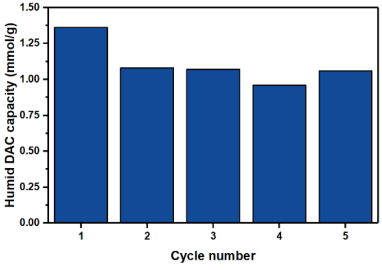
• Intermediate temperature required for effectively regenerating sorbents

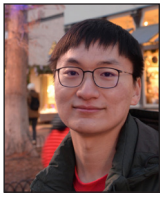
Recent Accomplishments

• Developed a highly porous metal hydroxide to efficiently and rapidly capture ambient CO_2 (> 1 mmol CO_2/g sorbent) under humid environment and can be cycled for 5 cycles under 150 °C

• Developed effective strategy to enhance the DAC performance by metal doping







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ChBE

Decarbonizing Steam-Methane Reforming: Electrification Via Joule Heating of Catalyst-Coated Wires

Research Themes

• Investigate the viability of Joule (resistive) heating of catalyst-coated high-resistance wires as a potential method for electrifying the heating process in steam-methane reforming (SMR)

• The global demand for hydrogen predicted to reach between 115-130 million tons by 2030. Bulk of this demand is driven by chemicals production and oil refining. The largest share of this demand comes from SMR.

Issues

• Unabated SMR is a significant source of greenhouse gas (GHG) emissions, a result of the use of natural gas combustion to supply the heat needed in SMR furnaces to drive the chemistry to high conversion.

• To reduce GHG emissions in the H2 value chain, the rapid development and deployment of large-scale, system-wide decarbonization measures are warranted.

Recent Accomplishments

• A reactor system consisting of a bench-scale electrified reformer using nickel/zirconia-coated wires was developed.

• Joule heating of a catalyst-coated wire is effective for SMR.

Elmer Ledesma

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ChBE

Thermal Modeling of Large Scale Liquid Hydrogen (LH_2) Storage Tanks

Research Themes

- Thermal conductivity models for cryogenic insulation materials
- Minimizing convection in the insulation layers of large-scale storage tanks
- Large scale non-vacuum tanks are needed to enable storage and transportation of LH_2

Issues

- Large property variation in cryogenic regimes leads to strong convective currents
- Multiple solutions exist for the same set of parameters

Recent Accomplishments

- Computed the critical points for avoiding convection in large scale cryogenic tanks
- Highlighted the change in solution behavior as a function of tank curvature

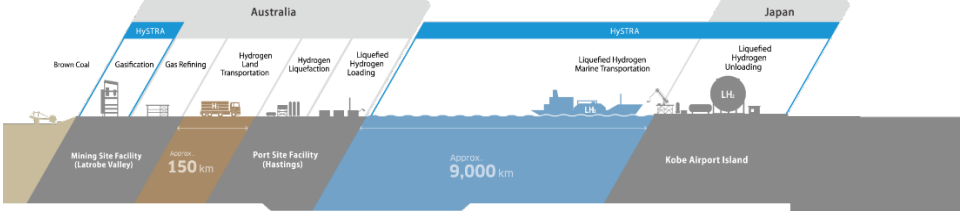

Fig. 1: HySTRA: An example of hydrogen supply chain

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ChBE

CULLEN COLLEGE OF ENGINEERING

ELECTRICAL & COMPUTER ENGINEERING

Deep Learning Enhanced Joint Inversion for Monitoring of Underground CO_2 Storage Sites

Research Themes

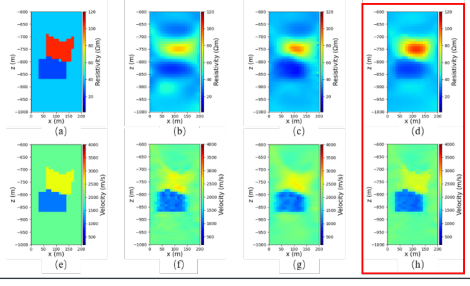
- Proposing a deep learning enhanced (DLE) joint inversion framework
- Applying to joint inversion of cross well electromagnetic data and seismic data
- Exploring extended applications in different scenarios

Issues

- Monitoring carbon dioxide (CO2) storage is crucial to tracking CO2 movement, evaluating storage integrity and early detection of CO2 leakage. However, the accuracy and flexibility of imaging the subsurface formation need to be improved.

Recent Accomplishments

- More accurate recovered property values and structural features than individual inversions and conventional cross gradient based joint inversion
- Excellent generalization on datasets using divergent geological structures
- Handling different sensing configurations
- Handling nonconforming discretization



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ECE

Motion Planning and Control of Underwater Robot

Research Themes

- Investigating magnetic sensing as an alternative for collision avoidance in underwater environments.
- Developing tailored algorithms and utilizing short-range magnetic sensors.
- Enhancing safety and efficiency in energy sector underwater operations.

Issues

- Generated a suite of simulations that test different magnetic proximity sensor configurations for obstacle avoidance and navigation.

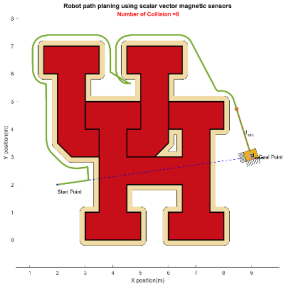
- Integrated simulation code with real sensors for advanced underwater collision avoidance research.

- Derived 2D ROV dynamic equations and designed a PID controller, advancing the field of underwater robotics and control systems.

Recent Accomplishments

- Limited sensor range restricts the application of more sophisticated navigation algorithms.

- Nonlinearity in ROV dynamic equations poses challenges in controlling the underwater vehicle effectively.



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ECE

Hydrogen Permeation in High-Carbon Steel

Research Themes

- Hydrogen permeation phenomenon
- Hydrogen permeation barrier (HPB) concept
- Room temperature synthesis of HPB and characterization

Issues

- Mitigation of hydrogen embrittlement and Hydrogen induced damage in high carbon steel
- Room temperature synthesis of HPB films-Chemical approach
- Development of characterization methodology

Recent Accomplishments

- Proof of concept for room temperature HBP synthesis
- Experimental apparatus for characterization (completed)
- Numerical analysis of data

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ECE

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MSE

Microwave-Plasma Assisted Methane Pyrolysis

Research Themes

- Utilize Microwave Plasma to assist with Pyrolysis of Methane
- Optimize 3D Catalyst Structure for maximum heating efficiency
- Negate need for catalyst swapping by eliminating buildup on structure with fiber design and material selection

Issues

- Sizing up for industry use goes against preferred designs of microwave reactors
- Carbon deposition inside reaction Area causing interference
- Building stable 3D structure requires more advanced deposition methods

Recent Accomplishments

- Successfully run small scale experiments with high conversion rates
- Have focused in on handful of catalyst designs to proceed with for in lab testing
- Vast collection of simulation work to provide clarification and guidelines for further development

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ECE

Analyzing Properties of Chitosan, PMMA & Cement

Research Themes

• Producing various composites of Chitosan with different percentage of Carbon then sintering for understanding the mechanical properties

• Re-cycling PMMA & it's various composites with different percentage of Carbon, casting & sintering for observing the mechanical properties

• Analyzing Cement & its composites with different percentage of Carbon for observing the mechanical properties

Issues

• In order to reduce particle size and forming great quality composites, milling needs to be done which is time consuming and a long process

• Mixing Polymer with Carbon and Cement to form composite did not show good outcome as it solidifies

Recent Accomplishments

• Remarkable results were obtained analyzing the mechanical properties of Chitosan and it's composites increasing the density, wettability and strength proving it can be good alternate of plastic

• Waste plastic was utilized and turned into different composites improves chracteristics when mixed with 1%,3%,5% Carbon

• Investigating properties of Cement shows how robust it can be with high density and strength having zero waste

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ECE

Navigation through Underwater Scaffolding using Magnetics

Research Themes

• Develop magnetic-based methods to detect metallic objects underwater

• Implement controllers to avoid detected metallic objects

• Improve robotic underwater navigation by complimenting traditional methods, like acoustics and optics, with magnetics

Issues

• Effect of metallic objects in a magnetic field is complex to solve analytically

• Commercially available metal detectors are limited in range, less than half a meter

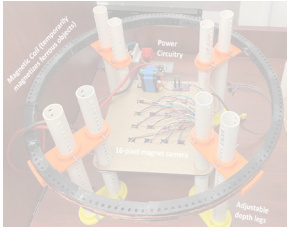
• Underwater testing requires a lot of preparation (waterproofing, topside communication, etc.)

Recent Accomplishments

• Our current prototypes can successfully detect metal objects up to ¬20[cm] away in air. Newest prototype includes amplifiers that could further increase range

• Metal objects can be detected and roughly tracked using commercial magnetic sensors

• Controllers have been implemented and tested using simplified computer simulations



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ECE

Physics-informed Deep Learning-based Surrogate Models for Accelerated CCUS Modeling – Towards Net Zero Carbon Emissions

Research Themes

- Developing Physics-informed Deep Learning-based Surrogate Models
- Accelerating CCUS Modeling and Decision-Making
- Addresing Challengs in CCS Decision-Making

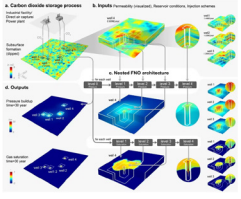
Issues

- Stochastic high spatial resolution simulations of CO_2 plume migration in subsurface are limited by computational resources. History matching, sensitivity analysis, and uncertainty quantification of CCUS modeling to support the scale-up of CCS deployment

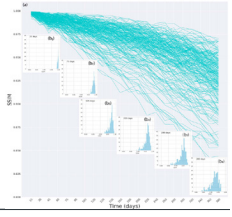
- Optimal CO_2 Injection Site Selection: Exploring efficient algorithms for selecting optimal CO_2 injection sites in CCS operations. Storage Efficiency and Pressure Control: Addressing challenges in improving storage efficiency and controlling pressure buildup during CCS processes.

Recent Accomplishments

- Developed Physics-Informed Surrogate Model: Successfully designed and implemented a deep learning-based surrogate model for CCS simulations. Incorporated domain knowledge and physics-based constraints into the model to enhance accuracy.



- Accelerated CCS Simulation: Achieved a significant (1000x) acceleration in simulating CO_2 plume migration compared to traditional numerical simulators. Conducted real-time assessments of CCS scenarios, allowing for faster decision-making processes.



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ECE

Detection of Metal Objects Using Magnetic Fields

Research Themes

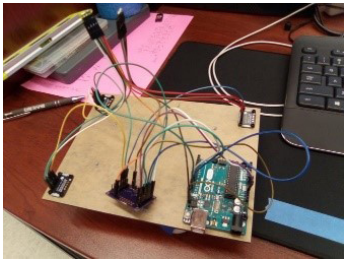
- Visualization of Magnetic Field Deflections
- Identification of Nearby Conductive Objects and their Locations
- Scanning an Area of Conductive Objects

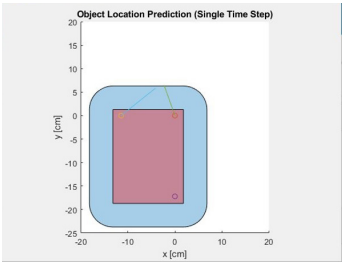
Issues

- Ambient Magnetic Interference Blurs Readings After 15cm
- Different Conductive Objects Deflect at Different Magnitudes
- Hardware Can't Interpret Rotation Yet

Recent Accomplishments

- Expandable Multichip Interface Implemented
- Triangulation Averages Out Errors for Consistent Location Predictions
- "Dry Test ROV" Constructed and Interfacing





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ECE

Toward AI-guided Catalyst Screening for Hydrogen Production

Research Themes

• Implementation of high-throughput synthesis and screening of catalyst using robotic arm & conveyor systems to moves sample through processes.

• Using Optical methods including our latest RIM imp technology to determine the quality of synthesized catalysts (mainly electrodeposition).

• Using Machine-Learning algorithms to determine the conditions of best catalyst from the datasets available from optical and performance characterizations.

Issues

• Conventional catalyst synthesis and characterization techniques involves longer time and resource consumption. Such high-throughput synthesis and characterization techniques can save a lot of time, resources and avoid errors due to human intervention.

Recent Accomplishments

• Shi, Y., Feng, G., Li, X., Yang, X., Ghanim, A. H., Ruchhoeft, P., ... & Shan, X. (2021). Electrochemical impedance imaging on conductive surfaces. *Analytical Chemistry, 93*(36), 12320-12328.

• Katirci, R., & Danaci, K. I. (2023). The optimization of nickel electroplating process parameters with artificial intelligence methods. *Journal of Applied Electrochemistry*, 1-13.

• Fatehi, E., Thadani, M., Birsan, G., & Black, R. W. (2023). A Critical Evaluation of a Self-Driving Laboratory for the Optimization of Electrodeposited Earth-Abundant Mixed-Metal Oxide Catalysts for the Oxygen Evolution Reaction (OER). *arXiv preprint arXiv:2305.12541*.

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ECE

Operando Imaging to study the Interfacial Reaction on Battery Electrodes

Research Themes

• Development of fast reliable and low-cost techniques for the characterization of energy storage devices

• Understanding Battery Solid Electrolyte Interface Formation using in situ Optical Imaging Techniques

• Study of safety parameters in solid state batteries, for the development of robust all solid-state battery chemistries at extreme conditions

Issues

• Cell level phenomena like intercalation, solid electrolyte interface (SEI) formation, lithium plating, involve complex interactions of electrochemistry and transport that are difficult to isolate. The occurrence of lithium plating depends on temperature, charge rate, state of charge, and electrolyte properties. Isolating each of these phenomena is challenging.

• Simulating operando conditions of a cell while maintaining an optical window for imaging

Recent Accomplishments

• Development of operando Reflection Interference Microscopy (RIM) Technique with high sensitivity as well as high temporal and spatial resolution- Studied In-situ formation of SEI in anode less Lithium Metal Battery (LMB)
Feng, Guangxia, et al. Nature Nanotechnology (2023)

• Development of stable imaging setup, that provides constant pressure and temperature for the operando imaging of Solid State Battery

• Visualization of Charge and Discharge process of NMC cathode in an all-solid state battery

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ECE

A Mobile Platform for Multi-modal Detection and Montoring of Methane Emissions

Research Themes

• By combining imaging solutions, such as infrared sensors and LiDAR, and chemical sensors, both spatial information and characterization of chemical agents can be identified.

• Deploy an affordable and intelligent monitoring system to collect the data and facilitate the detection task.

• Design and implement a feasible approach by using the mobile platform for the multi-modal detection of chemical threats and hazardous air emissions.

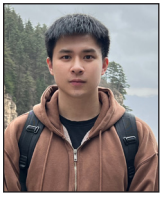
Issues

• Early and prompt detections are primary defensive actions to address concerns over chemical agents attacks and leaking hazards. Accurate and automated detections are pivotal for initiating rapid responses before they contact people.

Recent Accomplishments

• We have developed a multifunctional wireless communicated sensing and sampling box that can be carried by the drone for chemical fire plume detection.

• We have implemented the PhyDNN on a FPGA platform to reduce power consumption and produce accurate result by conducting forward DNN inference in real-time and explore its feasibility for an embedded system.



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ECE

Hydrogen and Battery-Based Hybrid Energy Storage System (ESS) for Future DC Microgrids

Research Themes

- Energy Management System
- Hybrid (Battery + Hydrogen) Storage System
- Power Electronic Converters

Issues

- The actual power grid is not fully capable of taking advantage of the high penetration of RES, making ESS the best solution to manage the power grid instability and balance supply and demand
- Integration of power electronic and fuel cell technology to seamlessly store and convert Renewable Energy Resources (RES) into electricity

Recent Accomplishments

- Won third place at the first America-Made Carbon Management Collegiate Competition hosted by the U.S. Department of Energy's Office of Fossil Energy and Carbon Management (FECM) for the concept of an optimized carbon dioxide transportation pipeline for the Houston Area.

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ECE

Novel Wireless Communication and Power Transfer System for Long Term Monitoring of CO_2 Seqestration

Research Themes

- Build toroid coil antenna wireless model.
- Channel capacity calculation.
- Wireless power efficiency calculation.
- Energy efficiency calculation.

Issues

• This system needs robust battery or super capacitor in extreme conditions for a long time.

Recent Accomplishments

• Energy efficiency calculation

• Different influenced factors study

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ECE

CULLEN COLLEGE OF ENGINEERING

CIVIL & ENVIROMENTAL ENGINEERING

Reviving Absorbent Chemistry of Amine For Improved Regeneration in Carbon Capture

Research Themes

- Electrochemical Carbon Capture-Climate Change Mitigation Technology
- Electrochemical Mediated Amine Regeneration (EMAR)
- Capturing Point Source Emissions i.e., Power Generation

Issues

- Kinetic Imbalance between Copper Oxidation and Reduction in EMAR
- Stability of Electrodes for Longer Operations
- Higher Energy Requirement at Lower Current Density

Recent Accomplishments

- Major Reduction in Charge Transfer Resistance by Employing Mixture of Amine
- Development and Testing of Continuous Bench Scale EMAR Cell for Flue Gases
- Reduction in Regeneration Energy

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CIVE

Electrochemical Processes for Direct Ocean Capture

Research Themes

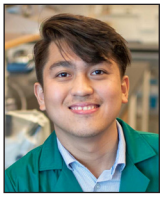
- Electrochemical Direct Ocean Capture (eDOC) for CO_2 reduction
- Developing methods for removing dissolved inorganic carbon (DIC) from the ocean
- Advancing sustainable negative emissions technologies (NET) for climate change mitigation

Issues

- Requires the use of expensive electrode materials such as platinum
- Operating current density not high enough for large scale carbon removal
- Need for fouling-prone ion-exchange membranes to facilitate operation of the electrochemical cell

Recent Accomplishments

- Novel modular and continuous electrochemical cell design without membranes
- Formulation of comprehensive theoretical model for efficient DIC removal
- Exploration of inexpensive and environmentally benign electrode materials and configurations



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CIVE

Transient Friction of Granular Material in Fault Shear Zones

Research Themes

• Understanding the sources of rate- and time-dependency in the sliding friction of fault shear zones

• Investigating the controls of the transient frictional behavior of granular materials under perturbations in sliding velocity and under stress relaxation processes

Issues

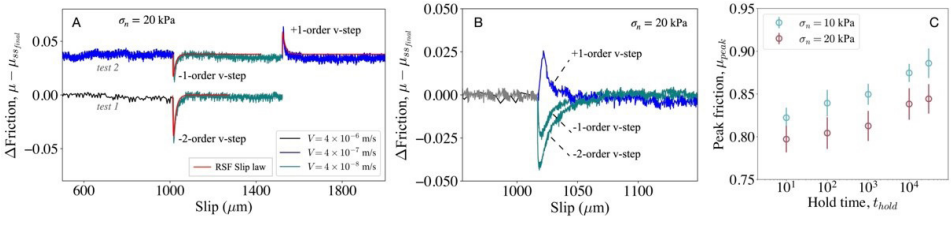
• It is not currently well understood what mechanisms cause the transient frictional response of fault rock and similar shear zones

• These shear zones are filled with granular materials. However, the contribution of granular physics to their frictional behavior has not been previously quantified in well-controlled experiments.

Recent Accomplishments

• I performed rheology experiments (velocity-steps and slide-hold-slides) on idealized and synthetic granular materials (silica powder and glass microspheres) as well as on geological materials at low confining stresses and low sliding velocities.

• The transient friction parameters and response form of the granular materials at low pressures are similar to those measured for earthquake fault shear zones.



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CIVE

Real-time Forecasting of Thermal Drawdown in Geothermal Systems Using Physics-Informed Neural Networks

Research Themes

• Develop a physics-informed neural networks model to efficiently integrate geothermal data and predict the thermal properties accurately.

• Model validation using DOE's Geothermal Data Repository.

• Accurate predictions of thermal power production of enhanced and advanced geothermal systems.

Issues

• Environmental pollution resulting from the excessive utilization of carbon-emitting oil and gas.

• Increasing demand of oil and gas leading towards low-carbon energy solution.

• Necessity of clean energy resource

Recent Accomplishments

• Worldwide advancement of a low-carbon energy solution: Enhanced Geothermal Systems (EGS). Example: Joint venture of Chevron and Baseload Capital.

• Worldwide popularity of Advanced Geothermal Systems (AGS) for even more cost-efficient geothermal systems. Example: A joint collaboration of Chevron New Energies Japan and MOECO to conduct tests on ACL.

• Recognition of EGS and AGS as the potential source of clean and renewable energy by the US Department of energy.

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CIVE

Free-volume Engineering of Polyamide Desalination Membranes by Incorporating Contorted Monomers

Research Themes

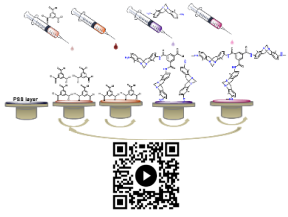
• Overcoming the permeability-selectivity tradeoff in conventional polyamide desalination membranes by incorporating shape-persistent, “contorted” diamine monomers to increase polymer network free volume.
• Controlled assembly of contorted polyamide films with tunable thicknesses through molecular layer-by-layer deposition.

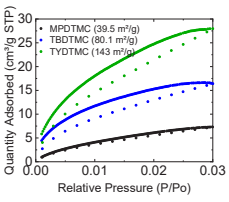
Issues

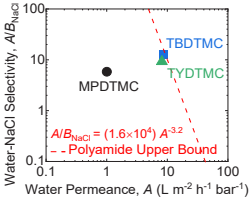
• Solution-diffusion modeling of water and salt transport to better understand the relationship between polyamide free volume characteristics and permeability-selectivity.
• Scalability of the molecular layer-by-layer synthesis of contorted polyamide films remains a challenge.

Recent Accomplishments

• Incorporating contorted TBD and TYD monomers into polyamide membranes increases network free volume compared to conventional MPD polyamide.
• Contorted TBDTMC and TYDTMC polyamide membranes exhibit high permeability-selectivity. Water permeability increases while maintaining high salt rejection.
• Desalination processes may be intensified with contorted polyamide membranes by achieving higher water production at equivalent salt rejection, thereby improving system energy efficiency.







United States Provisional Patent Application 63/465,520

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CIVE

Interfacial Materials for the Energy Transition

Research Themes

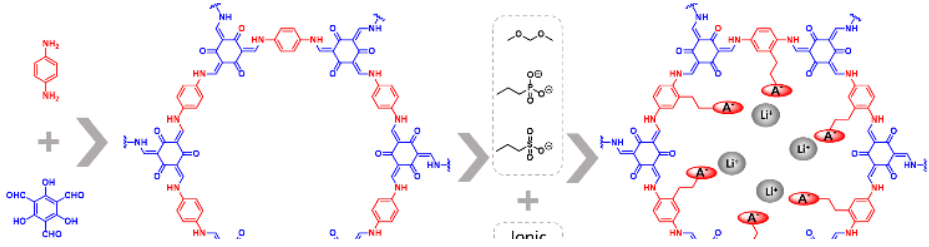
- Developing thin film membrane materials for selective ion transport
- Functionalizing Covalent Organic Frameworks (COFs) to selectively transport lithium ions and to host ion-selective media.
- Predictive modeling of single ion transport through interfacial materials

Issues

- Scalable processing of Covalent Organic Frameworks into thin film materials with controllable thickness.
- Selective transport of lithium ions in competitive environmental systems, especially aqueous solutions containing sodium and magnesium.
- Understanding of solvation behavior of ionic species at the membrane interface and quantifying energetic barriers to ion transport through membrane pores

Recent Accomplishments

- Applied thin film COF membranes as a functional battery separator to block soluble cathode species in an organic battery system.
- Incorporated ionic liquids with high lithium selectivity into the pores of covalent organic frameworks
- Tuned covalent organic framework membrane pore chemistry to increase lithium permeability.



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CIVE

CULLEN COLLEGE OF ENGINEERING

INDUSTRIAL ENGINEERING

Designing of an Equitable Community Microgrid

Research Themes

•Equity Metrics and Energy Justice

• Community Micro-grid

Issues

• The community microgrid definition is not very well defined in the literature.

• It is challenging to define new indexes that reflect the community's situation.

• Solving large scale optimization problems are hard and time consuming, specially mixed integer programs.

Recent Accomplishments

• Presenter at INFORMS conference 2022.

• Presenter at QPRC conference 2023.

• Presenter at THC conference 2023.

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IE

CULLEN COLLEGE OF ENGINEERING

MATERIALS SCIENCE & ENGINEERING

Upcycling of Polypropylene Mechano-Chemical Degradation

Motivation

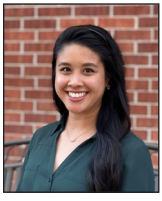
• Over 60% of plastic municipal solid waste are polyolefins and recycling rates for polypropylene are extremely low, < 5%.
• Polyolefin waste accumulates in oceans and landfills, with half-lives ranging from 58 years to 1200 years (HDPE).

Research Themes

• Previously, polypropylene pyrolysis has been widely studied to target useful liquid and gas products at temperatures greater than 400°C.
• Controlled pyrolysis procedures at low temperatures is used to induce mild degradation of polypropylene for an end-functional, recyclable solid residue.
• Combining thermal and mechanical energy can induce chain scission in the melt while maintaining mild degradation conditions.
• End-chain functionality from a degraded polyolefin is a promising route to waste upcycling and recycling. Functionalization can allow waste polyolefins to become compatibilizers or be copolymerized to make new materials.

Conclusions

• Solid residue collected from low-energy, mild pyrolysis has preserved high molecular weight compared to virgin polymer and shows end-chain functionality.
• Obtaining polypropylene residue with terminal vinylidene end groups allow for selective functionalization of linear chains as a promising method for upcycling.
• Residue functionality is linearly related to gas production. Then, the tradeoff for preserving high molecular weight in the residue is a lower concentration of functional end groups.
• Employing additional forces, such as ultrasonication, can maintain mild conditions and enhance control over solid residue molecular weight.



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MSE

Thermite Welding Optimization by Means of Mechanical & Ultrasound Vibration

Issues

• Railroads, the most used form of transportation of oil, are repaired using thermite welding. This is a low-cost and fast process but the final part has a high porosity concentration and other contaminants.

Recent Accomplishments

• We have been applying mechanical and ultrasound vibration to a cell that simulates molten steel with the objective of finding the conditions that will decrease the porosity in the material through a design of experiments.

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MSE

A Multifunctioning Highway System Incorporating Superconductor Levitated Vehicles & Liquefied Hydrogen

Research Themes

• Superconductor application

• Thermoelectric materials and Device

• Spent Lithium-ion battery recycling

• Water electrolysis

Highlights

• This work proposes the integration of multiple functions, such as the transport of people and goods, as well as energy storage and transport into one system.

• The entire system incorporates a superconductor guideway with the existing highway infrastructure, allowing for levitation of vehicles with magnetized undercarriages and lossless transmission and storage of electricity. Integrated liquefied hydrogen additionally allows for simultaneous cooling of the superconductor guideway and sustainable energy transport and storage.

• An experimental demonstration of a critical technical prerequisite for the proposed SCLev system: levitating a magnet above a superconductor guideway.

Recent Accomplishments

• A Novel Acid- and Base-Free Process for High-Yield Recycling of Lithium-Ion Battery Materials (patent)

• O. Vakaliuk, S. Song, U. Floegel-Delor, F. Werfel, K. Nielsch, and Z. Ren, APL Energy 1 (1), 016107 (2023).

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MSE

Induction Composed Frequency Heating

Research Themes

- Induction Heating
- Composed Frequency
- Gears Heat treatments

Issues

- Destructive Electromagnetic Interference
- Lack of homogeneous tempering

Recent Accomplishments

- Master in advanced technology

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MSE

Raman Spectroscopy for REBCO Characterization

Research Themes

• Developing a method of quality control (QC) for REBCO or High Temperature Superconductor (HTS).

• Characterizing REBCO structures, defects, degree of epitaxy, strain, etc.

• Acquiring database of different samples composition for prediction of material performance.

Issues

• Micro-Raman systems featuring high resolution have an inherent limitation in their speed due to small detection area.

• Defocus issues can result in loss of signal intensity leading to misfit of Raman peaks and misinterpretation of the data.

• Important to control tapes flatness for long lengths of REBCO tapes for reel-to-reel characterization applications.

Recent Accomplishments

• Tapes texture quality control capable of recognizing a-grains from c-grains growth.

• Tapes characterization of long lengths up to 1 m across the entire width 12 mm.

• Performance correlation between the retention factor and tapes strain.

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MSE

Molecular Origins of Aging of High Performance Polymers Under HPHT

Research Themes

- Molecular origins of Aging of Fluoroelastomer under HPHT conditions
- Molecular origins of Aging of Polyetheretherketone under HPHT conditions
- Simulated aging of amorphous Polyetheretherketone under HPHT conditions

Issues

- Studying degradation can help us find ways to limit or mitigate degradation of important macroscopic properties in Fluoroelastomer. Evaluation of Elastomer aging performance in HPHT zone (T>2000C, P>20 MPa) is not studied.
- The study offers a detailed molecular-level understanding of HPHT aging-induced changes in PEEK, shedding light on the critical roles of aging duration, temperature, and pressure in altering the material's mechanical and thermal properties.
- During experimental aging of PEEK, only the amorphous region was affected. Therefore, simulations were performed to further probe the amorphous region

Recent Accomplishments

- Comparison of aging environments (water and hydraulic) was successfully performed to highlight the differences in degradation mechanisms of FKM in each fluid.
- The implications of these findings are significant for engineering more robust and reliable PEEK materials. By understanding how the material behaves under HPHT conditions, we can optimize its performance and longevity in various critical applications, making PEEK a valuable material choice for extreme environments.
- The simulation findings offer important insights for designing and predicting PEEK's performance in HPHT applications. Understanding the complex degradation mechanisms can aid in developing more resilient and durable polymers.

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MSE

Manufacturing Scale-up of High Performance REBCO Superconductor Tapes

Research Themes

• Scale-up of the High Performance REBCO HTS tapes manufactured by A-MOCVD

• Decrease the unit cost of REBCO tapes ($/m) by refining processing methods and improving efficiency in converting precursor materials to superconductor film

Issues

• High cost of the HTS REBCO tapes

• Lower precursor conversion to film efficiency

Recent Accomplishments

• Successfully fabricated several 50 meter long REBCO tape by pilot-scale manufacturing tool with high critical current

• Coil fabricated with Advanced MOCVD tape and tested at 77 K and 65 K

• Demonstrated tape for DOE-AMO Next-generation Electric Machines (NGEM) Program, leads to 450 metric tons reduction of CO_2 emissions and $ 40,000 cost savings annually per superconducting motor

Chirag Goel

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MSE

Pet Coke-Derived Carbon for Advanced Solid-State Batteries

Research Themes

• Investigate the feasibility of producing carbon using pet coke as a precursor material.

• Develop the capability to customize the microstructure of carbon and assess its impact on the performance of solid-state batteries (SSBs) when used as an interlayer.

• Create an uncomplicated, cost-effective, and scalable method for producing nanoparticles.

Issues

• There is a requirement to devise a simple and scalable method for nanoparticle production that can also customize particle size and structure.

• The particle size of raw pet coke is too large to be used in the solid-state battery interlayer.

• The high sulfur content in raw pet-coke makes it unsuitable as an anode material for batteries.

Recent Accomplishments

• The sulfur content in pet-coke was successfully decreased from 4.4% to 1.6%.

• The particle size was effectively reduced from a few millimeters to the nanometric level.

• Nanoparticles were produced using the laser ablation technique, allowing precise control over the size of carbon particles.

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MSE

CULLEN COLLEGE OF ENGINEERING

PETROLEUM ENGINEERING

Electrokinetic and Electrodesposition Behavior of Asphaltene

Research Themes

• Determine the thermodynamic instability of asphaltene in heptane-toluene solution and crude oils
• Utilize laboratory setup in applying varied voltages for its deposition on electrodes
• Investigate the possible electrodeposition recoveries of asphaltene under different electric field strengths, electromagnetic exposure time, temperature, concentrations and polarities
• Using alternating voltages to alter the native charge of asphaltene

Issues

• Asphaltenes are characterized by being the heaviest fraction of crude oil, having high aromaticity, insoluble in alkanes, and soluble in light aromatic solvents
• However, asphaltene precipitation under changes in pressure, temperature and composition is a problem in downstream refinery operations when it fouls heat exchangers and is often mediated by laborious mechanical cleaning and expensive chemical dispersants
• Managing asphaltene deposition is a critical aspect of flow assurance. Therefore, the native charge of asphaltene provides the capacity to remove or prevent deposition by applying electromagnetic force

Recent Accomplishments

• Showed different electrokinetic behavior for +/- charged asphaltene
• Determined thermodynamic instability of asphaltene at heptol30
• Electromagnetic field strength is the dominant factor for electrodeposition
• Optimal electromagnetic field exposure time at 2mins above 4000 V
• 800V at 1.5cm electrode spacing for heptol80: lowest electrodeposition voltage (+ charged asphaltene)

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PE

Underground Storage in Salt Caverns

Research Themes

• Feasibility analysis of Hydrogen and CO_2 storage in salt caverns.

• Geomechanical modelling of the long-term response of the cavern and overburden strata to salt creep.

• Build a constitutive model to understand the creep and failure behavior of salt and its applicability to long-term CO_2 storage (990 years or more).

• Investigation of failure mechanism through elastoplastic modified Cam-Clay model with multistage triaxial tests, combined with finite element analysis.

• Reconsideration of the stability analysis of wellbores drilled into salt formations.

Issues

• The stress redistribution from CO_2 injection into a salt cavern might cause buoyant seepage through hydraulically conductive faults into shallow aquifers, reservoir compaction, and injection-induced seismicity.

• The deformation mechanism in salt caverns may result in various structural problems, such as subsidence, well casing deformation, and well integrity loss.

Recent Accomplishments

• Mapped out the Spindletop salt creep response at low deviatoric stress distally from the yield surface which showed only axial creep (1D response or zero lateral strain) having different strain amplitude scaling ratios.

• In contrast, the Spindletop salts showed equal strain amplitude scaling ratios both axially and radially at high deviatoric stress proximal to the yield surface (2D response or unconstrained boundary condition)

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PE

The Effect of Authigenic Carbonate Cement On Mechanical Properties of Mudrocks

Research Themes

• Seeking a method to chemically differentiate authigenic from detrital carbonate to develop models for predicting brittleness using bulk and trace elemental techniques in carbonate-rich mudrocks.

• Investigating the role of authigenic carbonate cement in the geomechanical property of carbonate-rich mudrocks.

• Researching characterization methods that allow direct correlation of micro-indentation mechanical properties with bulk mineralogy and acoustic microscopy.

Issues

• The volume and availability of authigenic carbonate cement should strengthen the rock and aid in better brittleness determination for carbonate-rich mudstone.

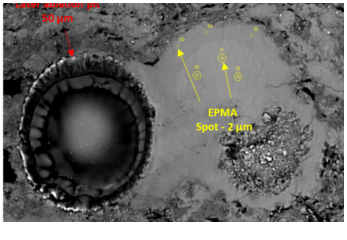
• Effect of cement on rock strength during multi-stage triaxial testing.

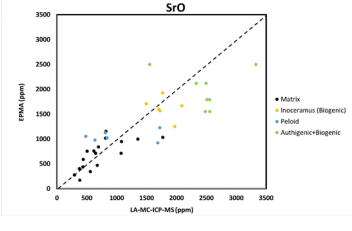
• Explore the existing gap between dynamic and static stiffness in mudrocks.

Recent Accomplishments

• Confirmed Sr, Fe, Mg, Mn, and Ba as proxies for authigenic carbonate cement.

• Upscaled geochemical proxies from nanometer to micrometer using two Microbeam analytical techniques. Determined proxy retention with upscaling.





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PE

Labratory Studies on Geochemical & Mineralogical Interaction between CO_2 Brine & Rocks for CO_2 Storage in Various Rock Formations

Research Themes

• This study examines the impact of CO2 sequestration on the geochemical properties and mineralogical structure of a saline aquifer on a lab scale.

• The gaps in knowledge are still there, in terms of experimental tests on CO2- rock- brine interaction, based on the impact of CO2-brine on the pore and grain geometry properties of rocks.

• The findings will contribute to understanding of how CO2 sequestration in deep saline reservoirs can be applied in practical scenarios.

Issues

• CO2 dissolving in brine can cause mineral dissolution in rocks, leading to mineral precipitation that clogs pore space and alter porosity and permeability of storage formation. Reduction in Permeability can cause decrease in injectivity and storage capacity.

• Brine acidification occurs when CO2 dissolved in brine and can create carbonic acid and lowering the pH of brine. It can also enhance the mineral dissolution, effects of the mineral release, and precipitation issues.

• Chemical reactions between CO2 and minerals in the rock can cause transformations or dissolution reactions that can affect the long-term stability of storage and the properties of the rock.

Recent Accomplishments

• We are selecting three rock types from US rock formations: dolomite, carbonate, and sandstone. First, we will measure critical properties (using YXLON FF20 CT SCAN, EDS- Energy-dispersive X-ray spectroscopy, FE-SEM Field Emission Scanning Electron Microscopes, IC Ion Chromatography, and ICP Inductively Coupled Plasma, XRD X-ray Powder Diffraction, and Helium Porosity meter) of the rock samples and composition of brine before and after SC CO2-rich brine injection using core flooding equipment.

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PE

Multiscale Characterization and Modeling of Conventional Reservoirs

Research Themes

• Characterizing the pore structure of carbonate and sandstone reservoir rocks using rate-controlled porosimetry and 2-D rock images.

• Developing digital rock models from 2-D rock images and rate-controlled porosimetry to accurately predict reservoir behavior.

Issues

• Comprehensive pore structure characterizing requires multiple experimental techniques and imaging modalities which can be expensive and time-consuming.

• Correlating pore structure heterogeneity at multiple scales remains a challenge.

Recent Accomplishments

• Built a rate-controlled porosimetry instrument with the highest known resolution.

• Developed a closure correction technique for rate-controlled capillary pressure measurements using wavelet transforms.

• Quantitatively described spatially correlated pore structure heterogeneity using the fractal dimension estimated from rate-controlled capillary pressure measurements.

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PE

Extended Aquifier System Pressure Behavior Under Carbon Storage

Research Themes

- CO_2 Sequestration
- Pressure Monitoring
- Plume Migration
- Aquifer Confinement

Issues

- Understanding of confined aquifers
- Long term CO_2 plume containment
- Pressure Monitoring and material balance

Recent Accomplishments

- Establishing aquifer selection fundamentals
- Developing long-term pressure monitoring
- Plume Modelling is extended systems.
- SPE ATCE 2023 Paper

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PE

Characterizing the Geomechanical and Geochemical Suitability of Saline Aquifers for Hydrogen Storage

Research Themes

• Effect of microstructure characteristics of siliciclastic reservoirs on geomechanical stability during cyclical injection/depletion of hydrogen.

• Impact of mineralogical alterations associated with hydrogen storage within sandstone reservoirs on storage integrity.

• Optimal criteria for selection of storage sites pertaining to siliciclastic reservoirs.

Issues

• Lack of field experience with underground storage of hydrogen in porous formations.

• Presence of potential risks associated with hydrogen storage in siliciclastic reservoirs such as: mineralogic alteration and geomechanical failure due to stress cycling.

Recent Accomplishments

• Development of a protocol for uniaxial-strain stress cycling to mimic cyclical injection/depletion of hydrogen.

• Development of a new image registration tool to provide a better understanding of the geomechanical responses of the given samples during stress cycling.

• Demonstration of geomechanical failure of coarse-grained, highly feldspathic sands to stress cycling.

• Demonstration of geomechanical suitability of fine-grained, quartzose sands to stress cycling.

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PE

Competitive Pricing of Hydrogen as an Economic Alternative to Gasoline & Diesel for the Houston Transportation Sector

Research Themes

• Competitive Pricing of Hydrogen as an Economic Alternative to Gasoline and Diesel for the Houston Transportation Sector

• Transportation Fuels

• Price Comparison

Issues

• The preference for liquid transportation fuels like gasoline and diesel relates to their much greater energy density.

• However, greenhouse gas (GHG) emissions from combustion of gasoline and diesel in the transportation energy sector account for 27% of US emissions.

Recent Accomplishments

• Compared three H_2 generation processes. The two processes that start with methane and water as feedstock are steam methane reforming (SMR) and SMR with carbon capture (SMRCC). The third process applies electrolysis using grid electricity and water as feedstock.

• Provided compelling evidence that gaseous H_2 would be competitive with gasoline and diesel for transportation in the greater Houston area.

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PE

Carbonate and Shaly Sand Petrophysics and Formation Evaluation

Research Themes

• Carbonate and Shaly Sand Petrophysics and Formation Evaluation.

• Developing the Thomas-Stieber method to differentiate the Structural and dispersed clay effect on the formation porosity.

• Using the Effective Medium approximation for the carbonate reservoir.

Issues

• The reading of the open hole well logs in the shaly sand are highly affected by the presence of the clay. The presence of clay may increase or decrease the porosity of the sand formation. Therefore, conventional well log interpretation may underestimate or overestimate the Hydrocarbon in place,

• The Carbonate reservoirs are characterized by the heterogeneity of their petrophysical properties. Different porosity types exist according to the depositional environment and the chemical change over time. Applying the Archie equation to Evaluate the hydrocarbon in place may have a lot of uncertainties.

Recent Accomplishments

• Adding a third axis to the Thomas-Stieber plot to derive an equation to separate the effect of all types of clay. The third axis is the velocity log data. The acoustic velocity varies according to the type of clay. It increases with increasing the dispersed clay and vice versa for the structural clay. Using this velocity property gives a big chance to estimate the accurate porosity.

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PE

EARTH & ATMOSPHERIC SCIENCES

GEOPHYSICS

Assessing Geothermal Potential in Eaglebine & Duvernay Basins

Research Themes

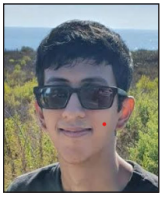
- Processing and cleaning raw data from oil and gas wells
- Using machine learning methods to estimate bottomhole temperature.
- Creating business model from perspective of an investor with a small capital

Issues

- Identification of 'energy need' regions by using different base map layers.
- Further investigation into economic impact by acquiring cost analysis for grid connection of power plants and geothermal surface facilities.
- While many wells have good geothermal potential, most do not satisfy all or most of the evaluation criteria.

Recent Accomplishments

- Developed machine learning models to calculate the geothermal gradient.
- Average Thermal Gradient of 25.5°C/km & 32°C/km for Duvernay and Eaglebine respectively suggests that both basins are good prospects for geothermal energy.
- Geothermal energy requires high volumes of flow, therefore, casing size, well capacity and age of the well are key factors to consider when repurposing oil and gas wells.



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GEO

Ultrasonic Measurements of Elastic Anisotropy of Granitic Rocks for Enhanced Geothermal Reservoirs

Research Themes

- Fluid Properties
- Shale oil and shale gas
- Elastic anisotropy properties
- Rock mechanics & geomechanics
- Seismic anisotropy Application
- Velocity dispersion & attenuation
- Potential seismic applications
- Rock physics modeling
- Log analysis and reservoir characterization
- Seismic forward modeling
- Seismic inversion workflow
- Machine learning fracture detection (Geothermal & GCS)
- Monitoring CO_2 Saturation and Geothermal fields

Issues

- Significant rock samples
- Laboratory machine and supplies issues
- Equipment update
- Licenses and software

Recent Accomplishments

- Knowledge and data about the pressure dependency of seismic waves and elastic anisotropies in granitic rock to enhance geothermal systems and monitoring.
- Comsol software license acquisition.
- Utah Forge geothermal field Core samples

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GEO

NATURAL SCIENCE & MATHEMATICS

PHYSICS
CHEMISTRY

Advanced Electrolyte Membrane for PEM Fuel Cell & Water Electrolyzer

Research Themes

• Developing highly durable proton exchange membrane (PEM) with reduced fuel crossover for proton exchange membrane fuel cell (PEMFC) and proton exchange membrane water electrolysis (PEMWE) using state-of-the-art perfluoro sulfuric acid (PFSA) based polymer known as NafionTM.
• Pore reduction is aimed on bench-marked chemically and mechanically stable, and durable in-house developed NafionTM-Plus and state-of-the-art NafionTM membranes by utilizing sulfonated dopamine through self-polymerization approach.
• Fabricating membrane electrode assembly (MEA) for validating the developed membranes in PEMFC and PEMWE specific.

Issues

• The radical generation via the gas crossover through the electrolyte membrane during PEMFC and PEMWE operation causes the reduction in cell performance and long-term stability. Thus, the reduction of gas crossover is an important factor while designing the electrolyte membrane.
• Especially in vehicular applications, membrane suffers from continuous hydration/dehydration cycle due to the fluctuation in current density. Hence, the electrolyte membrane should be dimensionally stable and mechanically strong.
• Low conductivity at elevated temperature and at low relative humidity.

Recent Accomplishments

• Successfully synthesized sulfonated dopamine as an additive in improved electrolyte membrane.
• Developed modified electrolyte membrane by self-polymerizing sulfonated dopamine into the NafionTM and NafionTM-Plus with enhanced mechanical property and proton conductivity.

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PHYS

A Universal & Quick Activation of Stainless Steel for Industrial Alkaline Water Electrolysis Application

Introduction

• Catalysts loading is widely used to prepare active electrodes for water electrolysis but usually suffers from weak connection between substrate and catalysts. In comparison, self activation has much stronger connection between catalysts and substrate. Stainless steel is extensively used in water electrolysis industry and contains active elements such as Fe, Ni, Cr, Mo and etc. Therefore, the self activation on stainless steel is a highly viable strategy to develop active electrodes for water electrolysis industry.

Methods

• Commercial available stainless steel mat (SSM, XL 2000) was utilized as conductive substrate.

• Heat treatment was first applied on SSM to increase the temperature.

• The heated SSM was quickly dropped into aqueous solution for quenching.

• After quenching, the SSM was fully activated for alkaline water electrolysis.

Recent Accomplishments

• **M. Ning**, L. Wu, F. Zhang, D. Wang, S. Song, T. Tong, J. Bao, S. Chen, L. Yu, Z. Ren, *Mater. Today Phys.*, 2021, **19**, 100419.

• **M. Ning**, F. Zhang, L. Wu, X. Xing, D. Wang, S. Song, Q. Zhou, L. Yu, J. Bao, S. Chen, Z. Ren, *Energy Environ. Sci.*, 2022, **15**, 3945-3957

• **M. Ning**, Y. Wang, L. Wu, L. Yang, Z. Chen, S. Song, Y. Yao, J. Bao, S. Chen, Z. Ren, *Nano-Micro Letters*, 2023, **15**, 157.

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PHYS

A Hybrid Approach to Hard Material Discovery

Research Themes

• Modified a machine learning model to predict load-dependent Vickers microhardness of materials (borides, carbides, silicides, etc.).

• Utilized Density Functional Theory (DFT) to calculate elastic properties such as bulk modulus (B) and shear modulus (G), offering insights into material hardness predictions.

• High-temperature synthesis to experimentally validate the machine learning model and elastic moduli-based predictions.

Issues

• B and G models fail to predict load-dependent hardness, leading to potential inaccuracies in material assessments.

• Composition-only models cannot differentiate materials like allotropes or polymorphs.

Recent Accomplishments

• Our machine learning model is more accurate on a robust dataset than the heavily cited elastic moduli models.

• The model led to the discovery of a novel, nearly superhard material (≥40 GPa @ 0.49 N load) published in the high-impact journal *Chemistry of Materials*.

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CHEM

Assembling a Solid-State Toolbox: Design Approaches for Complex Intermetallics

Research Themes

• Exploratory synthesis of polar intermetallics

• High-pressure crystal structure prediction via particle swarm optimization

• From simple to complex crystal chemistry in ternary gold systems

Issues

• The diversity of chemical systems and vast amount of possible materials remains beyond our capabilities. Highlighting the large number of new materials yet to be discovered.

• Crystal structure prediction of a solid state reaction is difficult if not impossible. Remaining one of the most fundamental challenges in solid state chemistry.

• Materials design with desired properties for specific applications represents a major challenge driven by the understanding of structure/property relationships and the complexity of experiments.

Recent Accomplishments

• Employed a comprehensive solid state toolbox that pairs experimental studies and computational models has proven effective for the systematic exploration of inorganic materials.

• Implementing pressure opens the door for the next generation of materials with unprecedented crystal structures and physical properties.

• Ultimate goal to develop reactivity principles via exploratory synthesis and computation for materials design.

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CHEM

LIBERAL ARTS & SOCIAL SCIENCES

POLITICAL SCIENCE

The Distributional Impact of State Climate Policies on Energy Burden, 2010-2019

Research Themes

• Household spending of more than 6% of its annual income on electricity is considered as experiencing a high energy burden

• Energy burden faced by low-income households is three times higher than those of other households

• Rapid, evolving, and constructive policy response across states has delivered promising climate results within a short timeframe

• However, the urgency to address climate change and its impacts can impose disproportionate costs and have unintended consequences for low-income groups

Issues

• Energy equity is central to mitigation policies that simultaneously address issues of energy and climate change

• RESEARCH QUESTION: What is the impact of climate policies across U.S. states on household energy burden – median energy burden and across income groups?

Recent Accomplishments

• The median energy burden increases with the scope and strength of climate policies; consistent across income groups. Low-income communities bear the most substantial impact, suggesting that climate policies across states have a regressive distributional impact

• Impact of climate policies on the energy burden for low-income communities is four times higher than for the median-income group

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PSCI

C.T. BAUER COLLEGE OF BUSINESS

FINANCE

Powering Tomorrow: Solar Panels & Molten Salt

Research Themes

• Solar panel advancements and innovations.

• Molten salt applications in renewable energy systems.

• Business plan development for solar panel technology, including financial and supply chain aspects.

Issues

• Enhancing the cost-effectiveness of solar panel production.

• Addressing potential environmental impacts of molten salt usage.

• Optimizing supply chain logistics for solar panel distribution.

Recent Accomplishments

• Explored novel solar panel designs for increased efficiency.

• Investigated the integration of molten salt in energy storage solutions.

• Developed a comprehensive business plan for solar panel manufacturing and distribution.

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FIN

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