Modular Reactors for Co-Generation of Liquid Chemicals and Electricity from Stranded Natural Gas

DE-FE0032235

Chuancheng Duan
Materials Research Lab for Sustainable Energy
Kansas State University

The University Training and Research (UTR) program

U.S. Department of Energy
National Energy Technology Laboratory
Resource Sustainability Project Review Meeting
April 2-4, 2024

Project Overview

– **Funding** (DOE Funding: $500,000, Cost Share: $0)

– **Overall Project Performance Date:** 06/01/2023-05/31/2026

– **Project Participants**

PI: Dr. Chuancheng Duan, Kansas State University

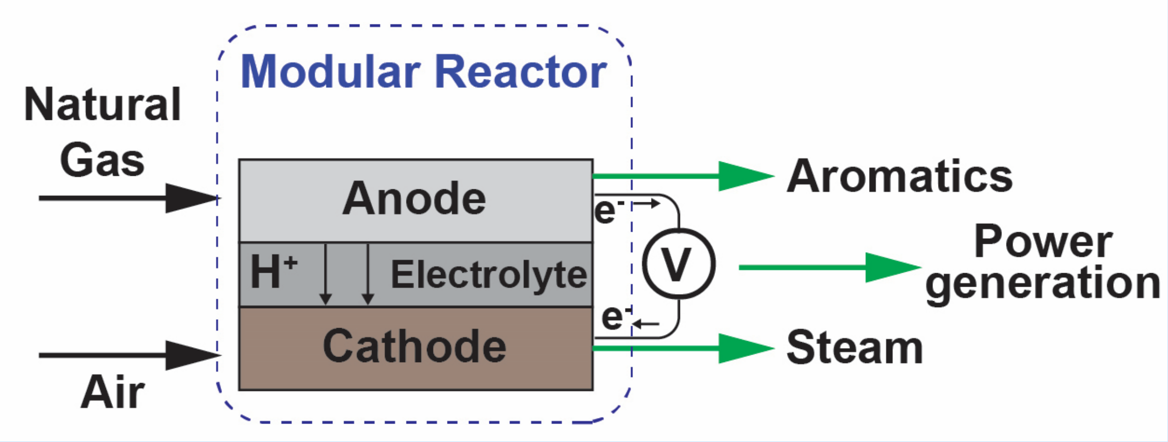
Co-PI: Dr. Pejman Kazempoor, The University of Oklahoma

Co-PI: Dr. Hanping Ding, The University of Oklahoma

Project Overview

Overall Project Objectives:

Design, demonstrate, and test a novel process-intensified modular system for natural gas (NG) upgrading to value-added liquid chemicals (aromatics) and power generation simultaneously.



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Project Overview

Overall Project Objectives:

Design, demonstrate, and test a novel process-intensified modular system for natural gas (NG) upgrading to value-added liquid chemicals (aromatics) and power generation simultaneously.

- The NG conversion and aromatics yield can be significantly improved by the enhanced reaction kinetics by electrochemically utilizing the hydrogen product for electricity generation.
- The proposed modular system aims to achieve NG conversion of >30%, aromatics yield of >50% increase, and >90% reduction in CO_2 emissions.
- The proposed project will educate and train the next generation of engineers and scientists, support early-stage research innovations, and equip the students with cutting-edge, translatable skillsets to succeed in longstanding and enduring careers.

Technology Background

Oil and gas fields

Landfill

Wastewater treatment facilities

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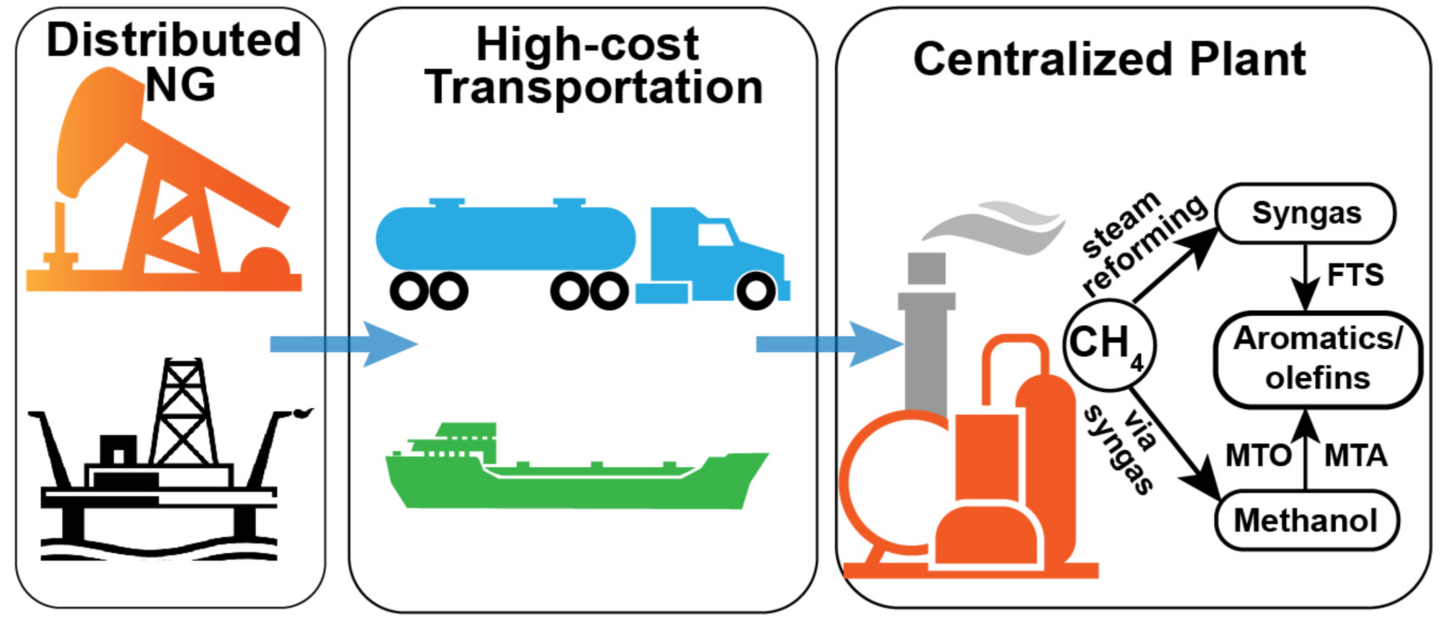
Technology Background



Conventional approaches to converting natural gas to high-value products

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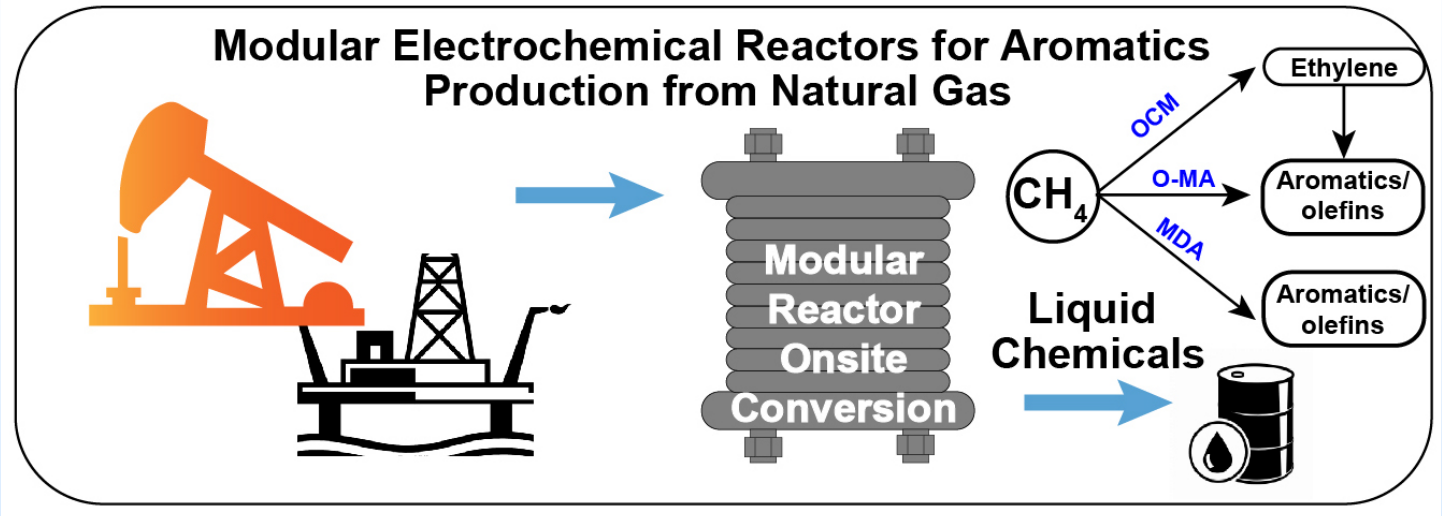
Technology Background



On-site conversion and utilization of methane using distributed and modular reactors could be the approach.

- **Minimized storage and transportation cost**
- **No flare**
- **Valorization of natural gas**
- **Mitigate emissions**

DMA/MDA (direct methane aromatization)

$6CH_4 = C_6H_6 + 9H_2$

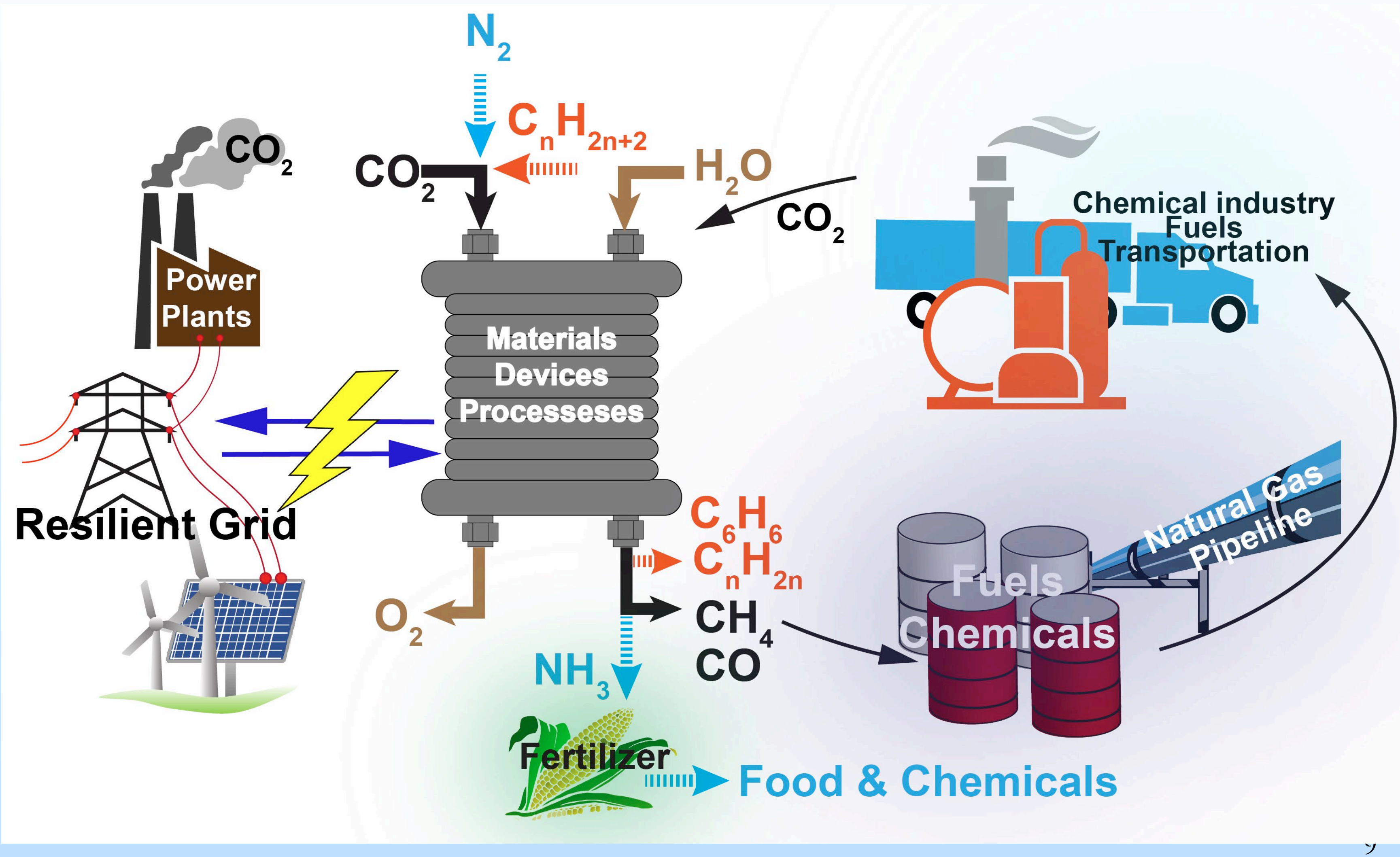
- Thermodynamically and kinetically limited
- High operating temperature
- Coking (i.e., carbon formation)
- Low conversion

Technology Background

$$6CH_4 = C_6H_6 + 9H_2 \quad \Delta G^o = 433 \text{ kJ/mol}$$

Liu, F., Ding, D., & **Duan, C*.** (2023) *Advanced Science*, *10*(8), 2206478.

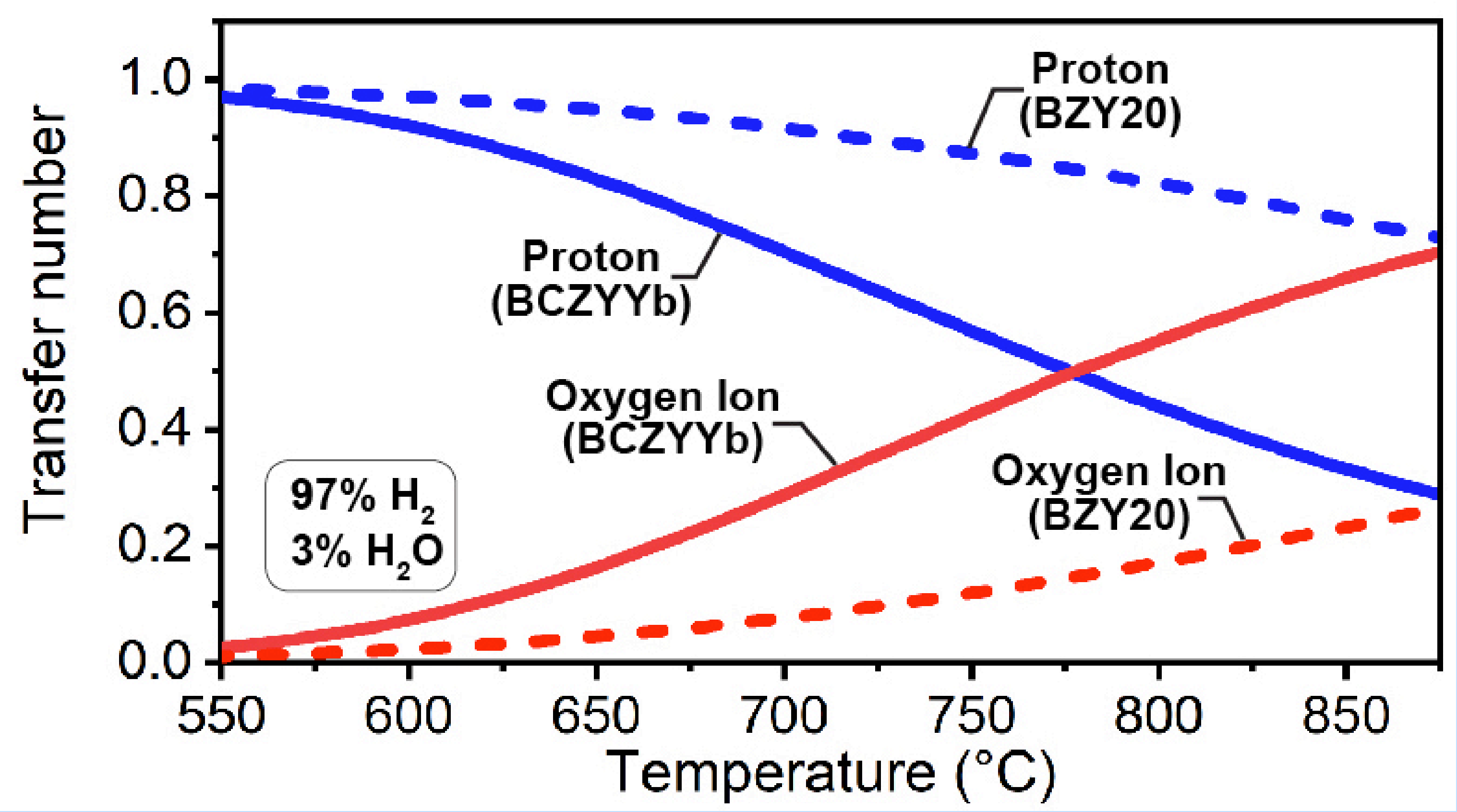
Technology Background



Liu, F., Ding, D., & **Duan, C*.** (2023) *Advanced Science*, *10*(8), 2206478.

Technology Background

Engineering the chemical compositions of $BaCe_{0.8-x}Zr_xY_yYb_{0.2-y}O_{3-\delta}$ (BCZYYb) to achieve mixed proton and oxygen-ion conductors

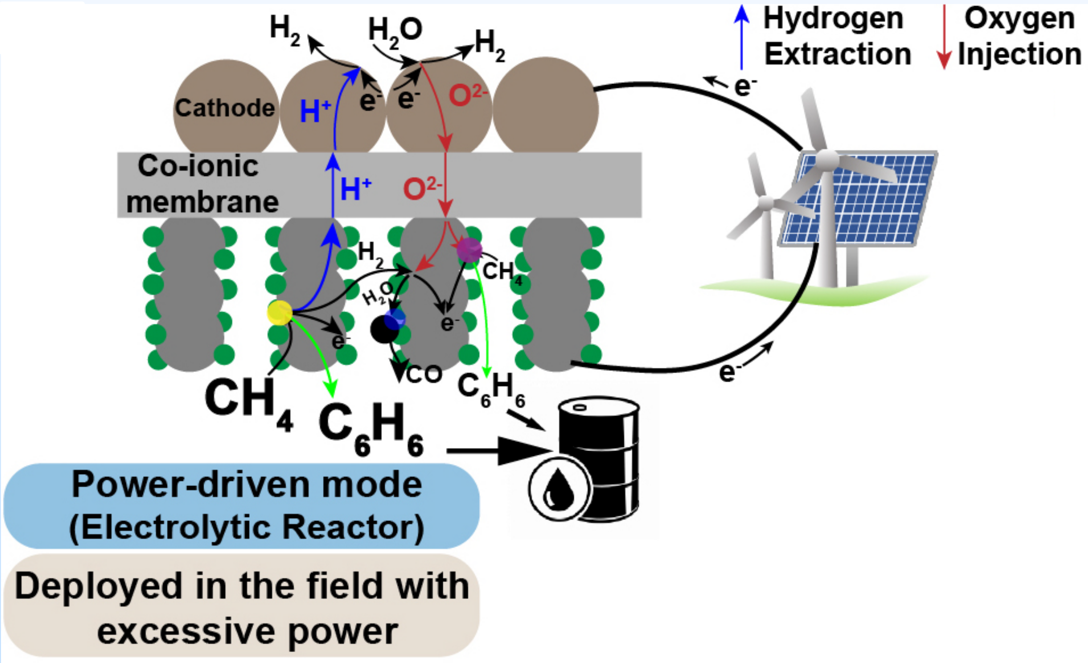


The ratio of proton flux to oxygen ion flux should be modulated to achieve high conversion, mitigate coking, and avoid over oxidation of reactants

Technology Background

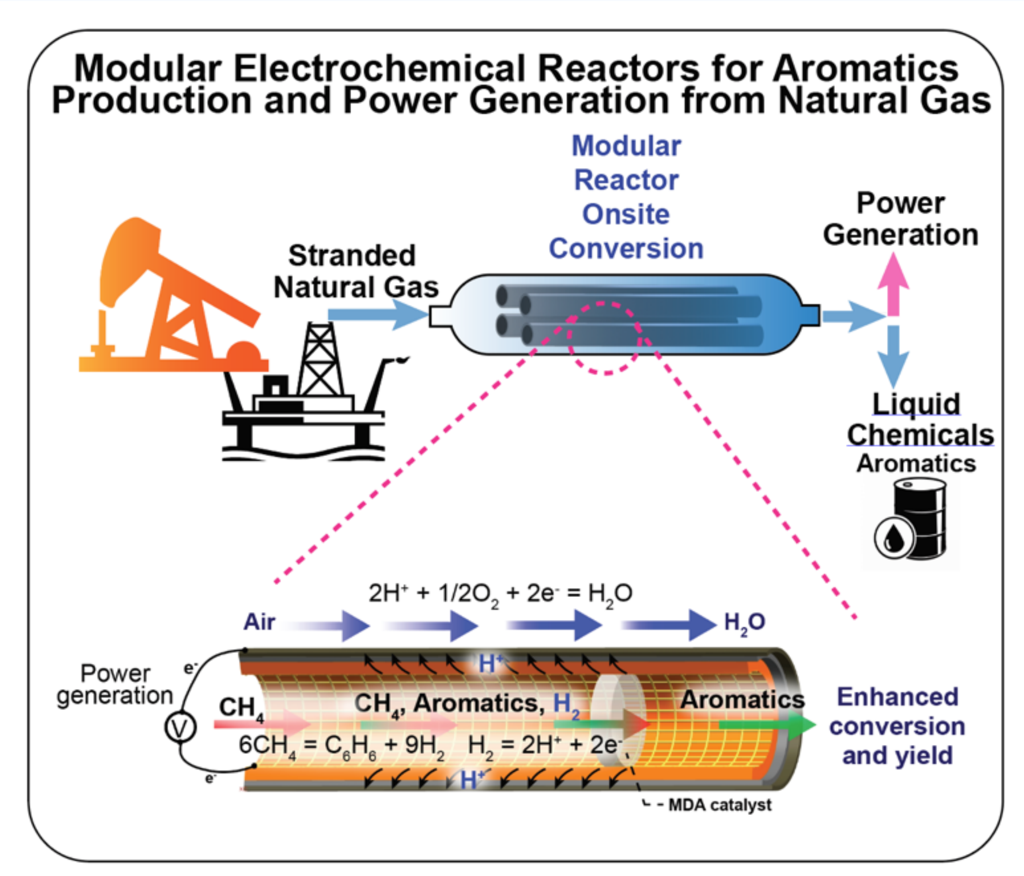
Electrolysis Mode

Fuel cell Mode



Liu, F., Ding, D., & **Duan, C*.** (2023) *Advanced Science*, *10*(8), 2206478.

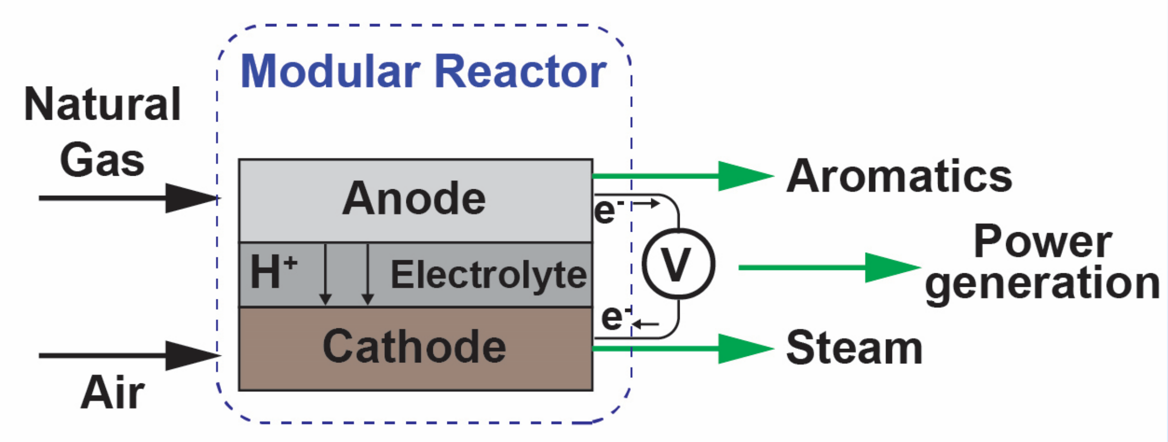
Technology Background



- ❑ Enhanced natural gas conversion
- ❑ Reduced aromatic production cost and GHG emissions.
- ❑ Co-generation of power.
- ❑ The coking and contaminants tolerant natural gas conversion catalyst enables durable operation.
- ❑ Simplified process and system and reduced capital cost.
- ❑ Maintain and upgrade the fossil fuel research and education capabilities at both KSU and OU.
- ❑ Support education and training of students

Technical Approach/Project Scope

Modular reactor for co-generation of liquid chemicals and electricity from stranded natural gas



Approaches

- ❑ Combine natural gas conversion, aromatization, and power generation.
- ❑ Manufacture tubular membrane reactors to enhance natural gas conversion and aromatics yield.
- ❑ Optimize the natural gas conversion catalyst and integrate it with the tubular membrane reactors.
- ❑ Computationally design and analyze the membrane reactors to guide system integration.

Deliverables

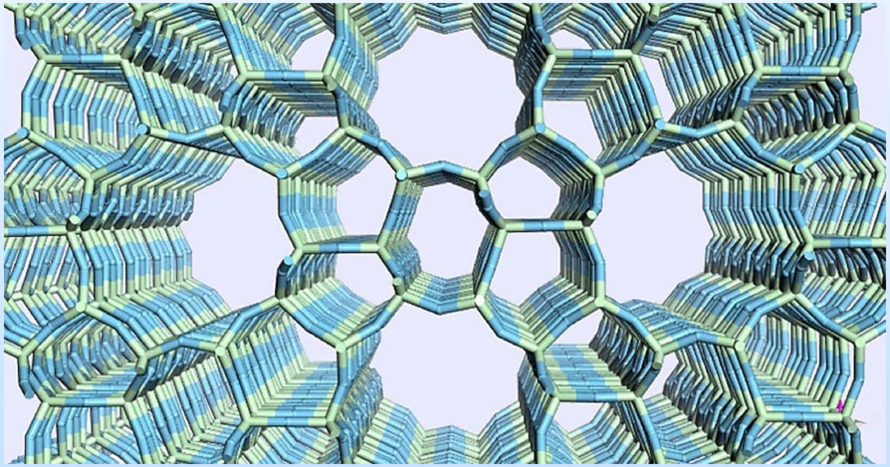
- ❑ Demonstrate intimately integrated reactors to co-produce aromatics and power from natural gas.
- ❑ Optimized materials for membrane reactors and natural gas conversion catalysts.
- ❑ Validated computational models and analysis results for this modular reactor.
- ❑ Education and train >6 students and scientists

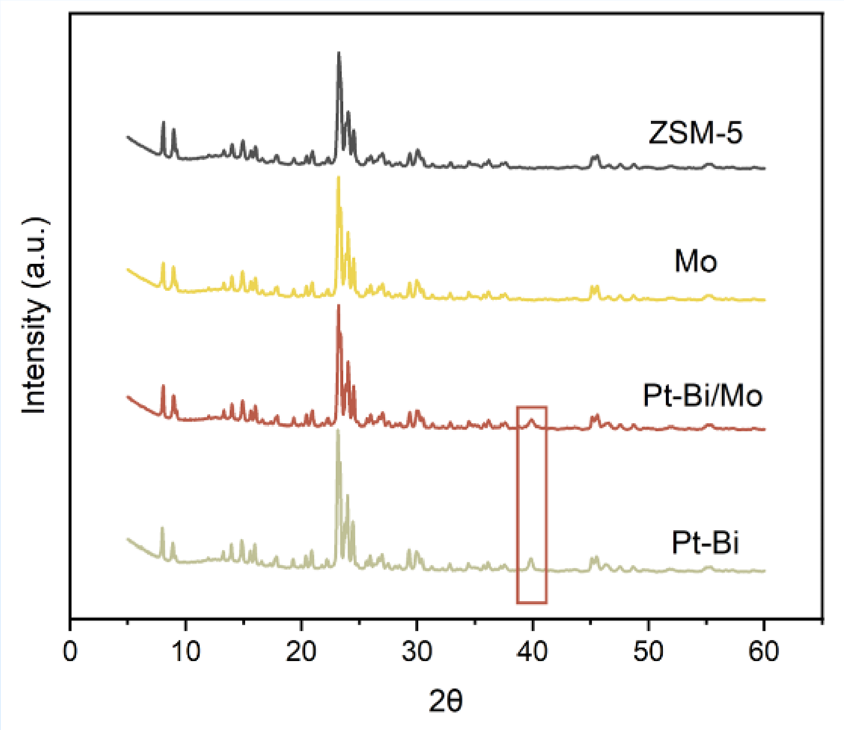
Technical Approach/Project Scope

Task name
Task 1 – Project Management and Planning
Task 2 – Establishing desired end states and identifying most suitable path from initial to end.
Task 3 – MDA catalysts development.
Task 4 – Fabricating and testing tubular PCEMRs.
Task 5 – System integration and process intensification to realize direct conversion of natural gas.
Task 6: Computational modeling of the proposed modular and process intensified system.
Task 7: Complete a comprehensive techno-economic and life cycle analyses of the natural gas conversion technology

Progress and Current Status of Project

Task 3- Methane Dehydroaromatization (MDA) catalysts development.





Novel tri-metallic Pt-Bi/Mo/ZSM-5

Unpublished results

Progress and Current Status of Project

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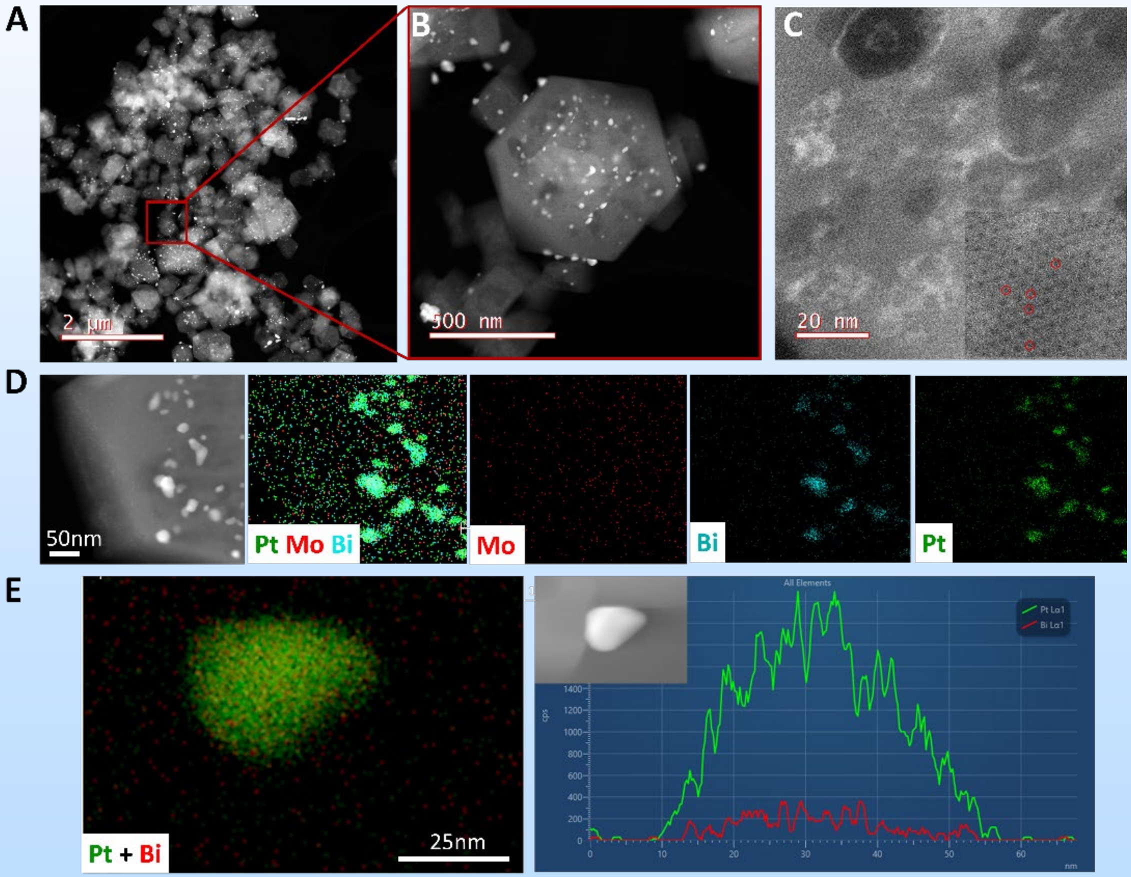

Unpublished results

Novel tri-metallic Pt-Bi/Mo/ZSM-5

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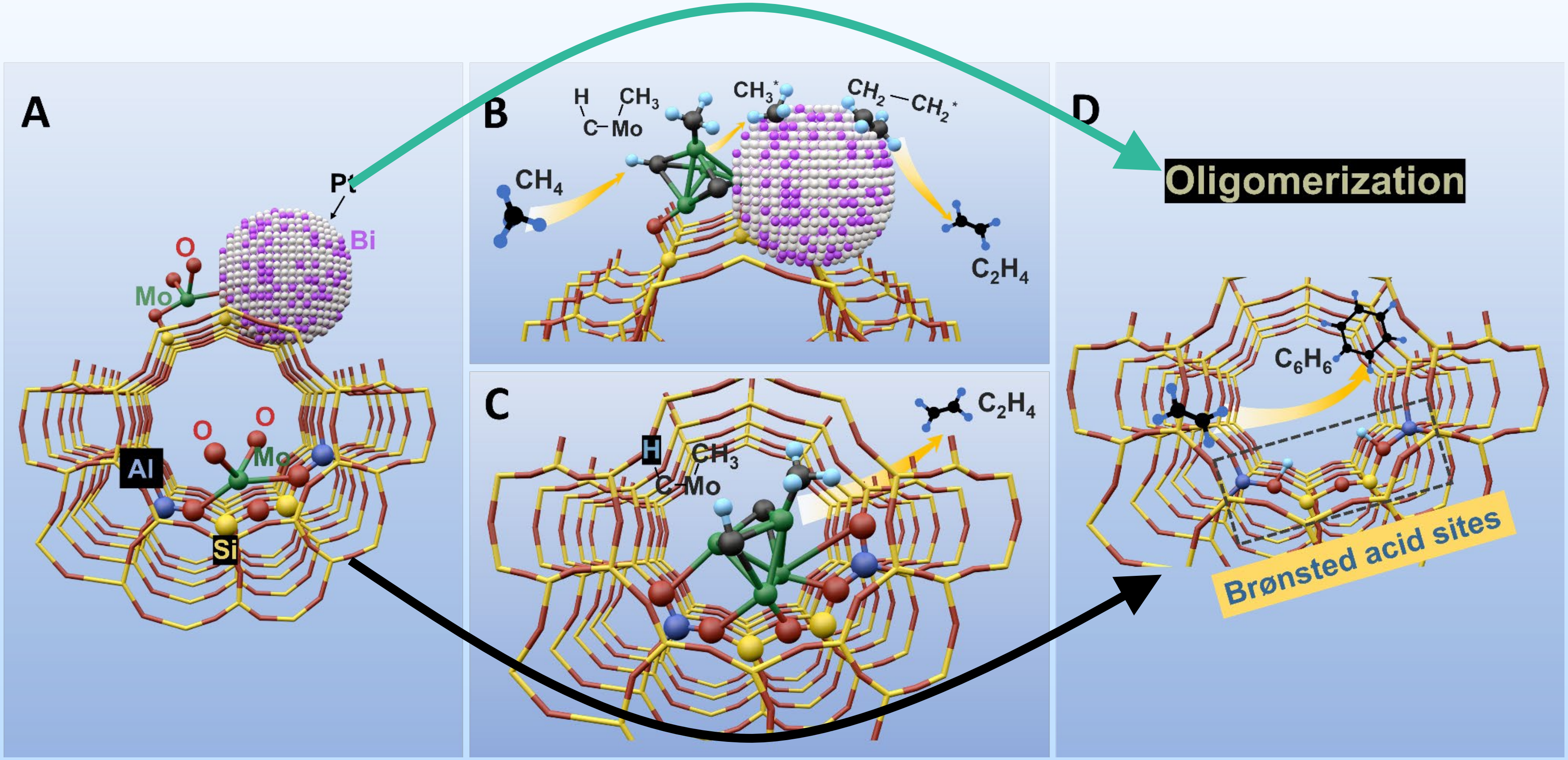
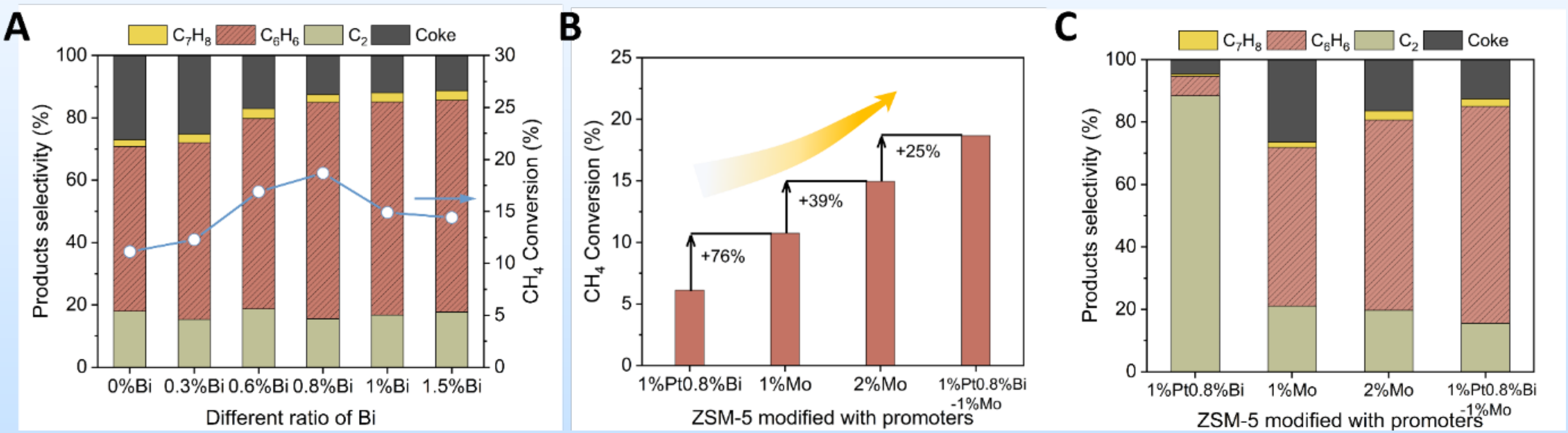


Novel tri-metallic Pt-Bi/Mo/ZSM-5 changes the reaction pathway

Unpublished results

Progress and Current Status of Project

Task 3 - Methane Dehydroaromatization (MDA) catalysts development.

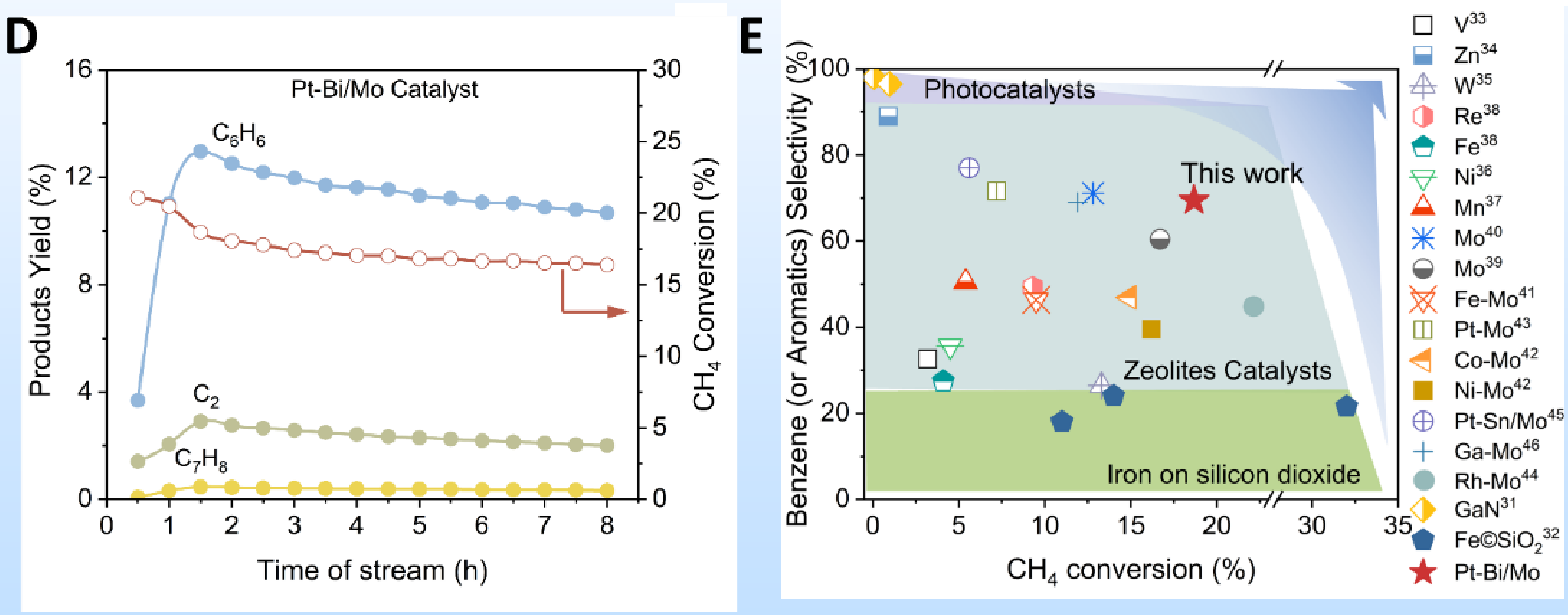


The tri-metallic Pt-Bi/Mo/ZSM-5 improves both CH_4 conversion and selectivity to aromatics

Unpublished results

Progress and Current Status of Project

Task 3 - Methane Dehydroaromatization (MDA) catalysts development.

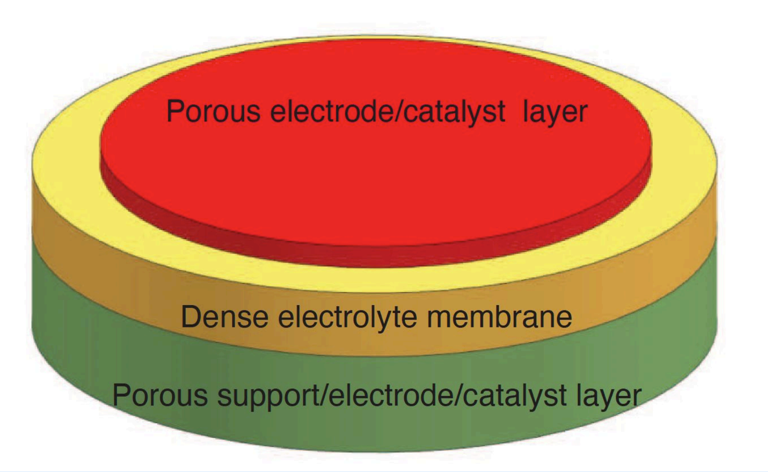


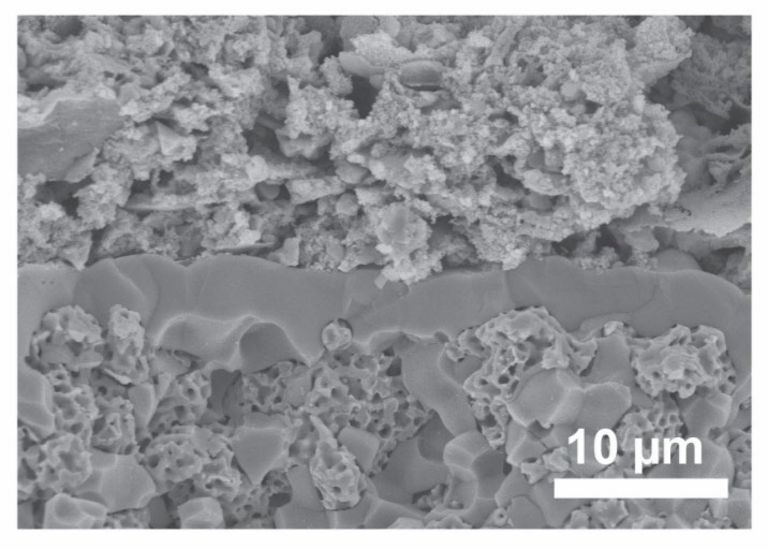
Both high CH_4 conversion and selectivity to aromatics are achieved on the new catalyst

Unpublished results

Progress and Current Status of Project

Task 4 – Reactor design, fabrication, and characterization.





Progress and Current Status of Project

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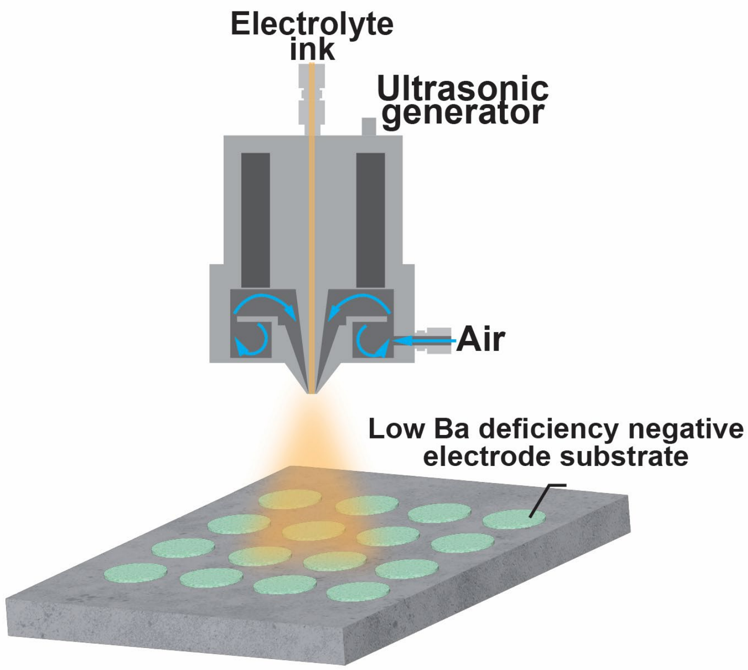
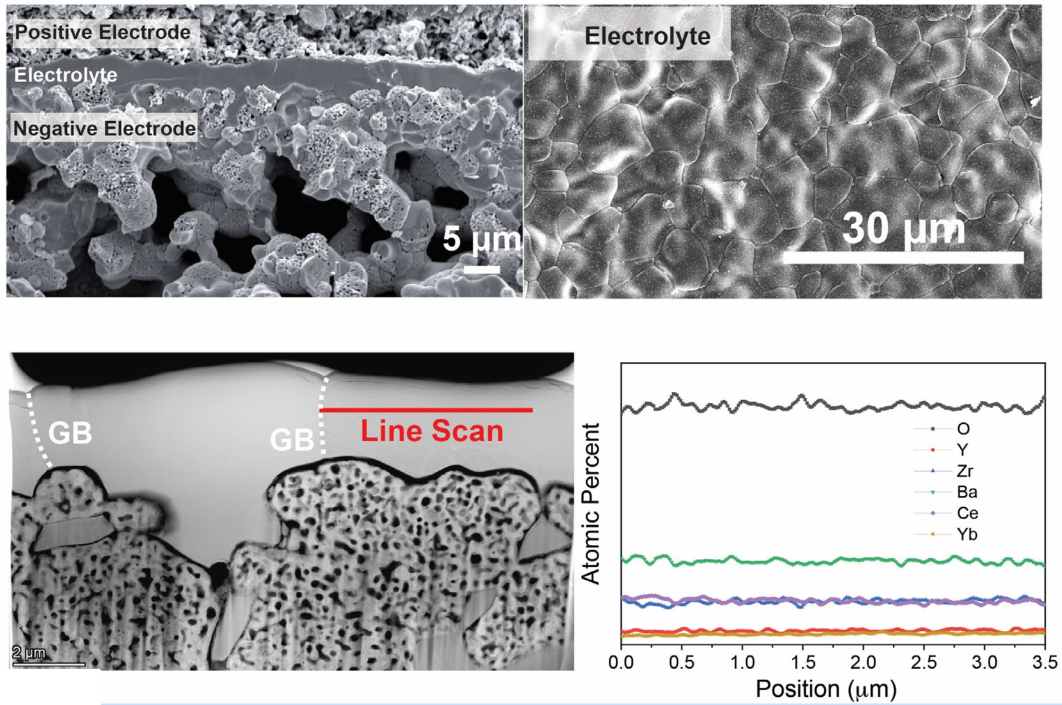


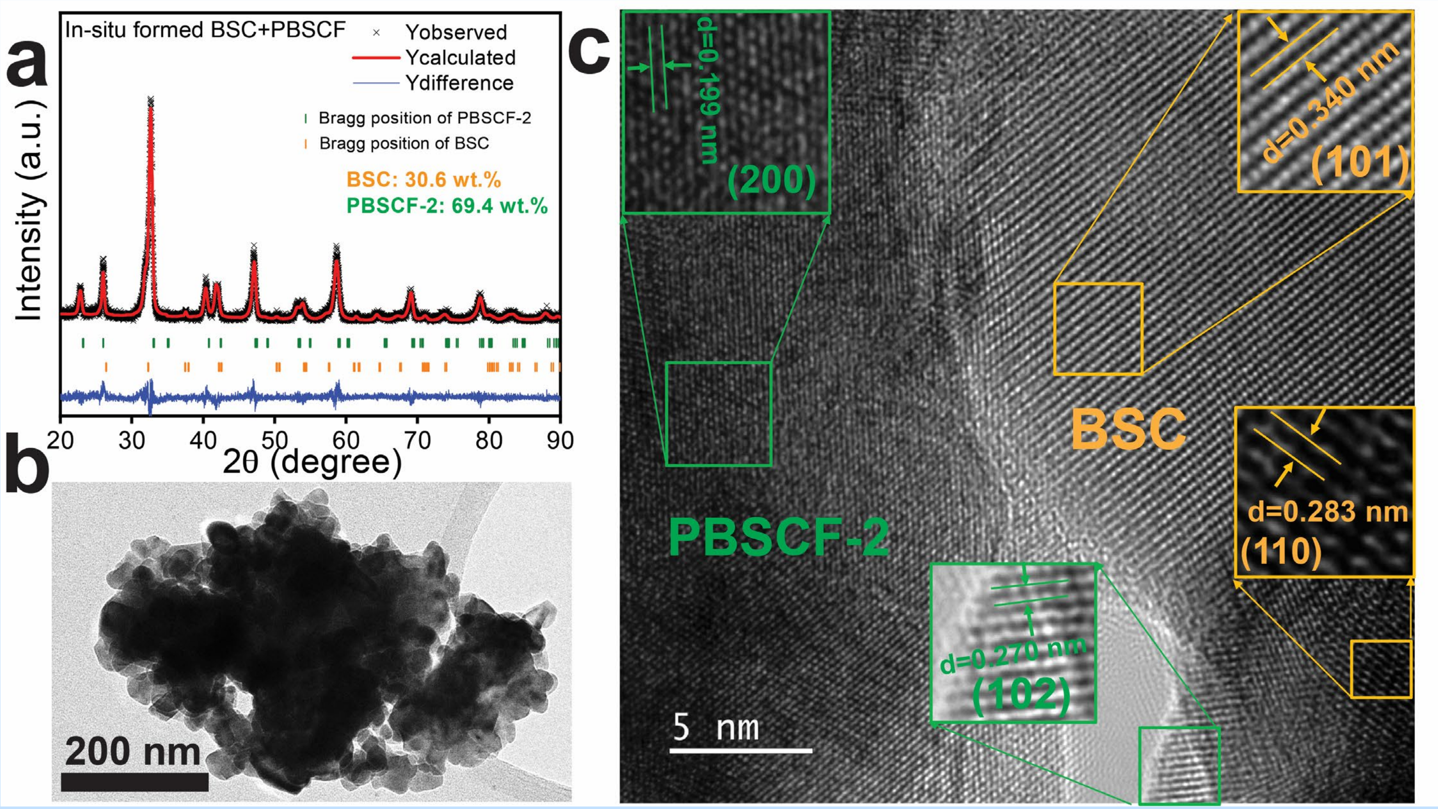


Advanced electrolyte materials and manufacturing process for reducing ohmic resistance

Liu, F, Duan, C et al. Nature Energy 8.10 (2023): 1145-1157.

Progress and Current Status of Project

Task 4 – Reactor design, fabrication, and characterization.

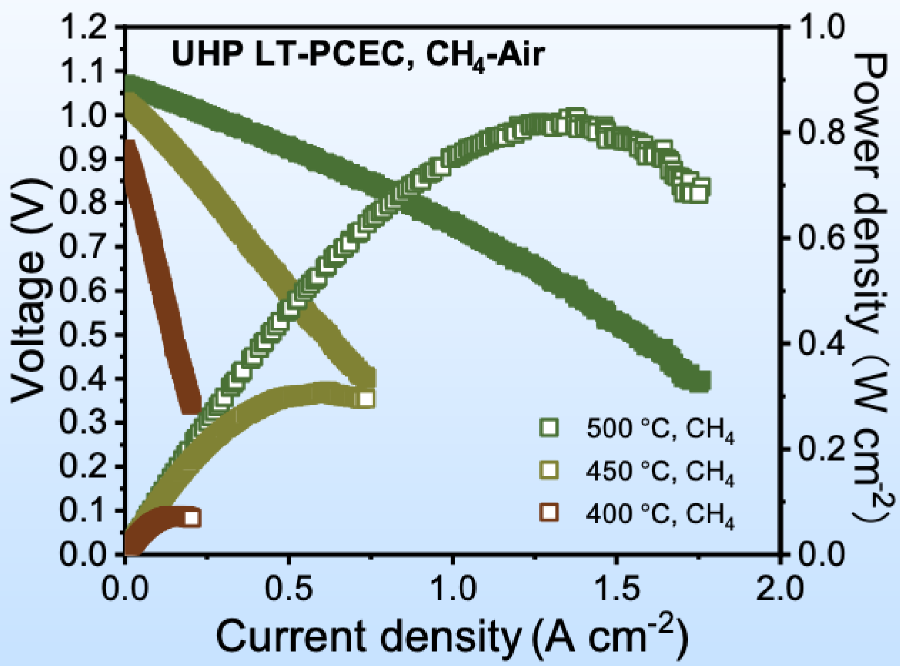


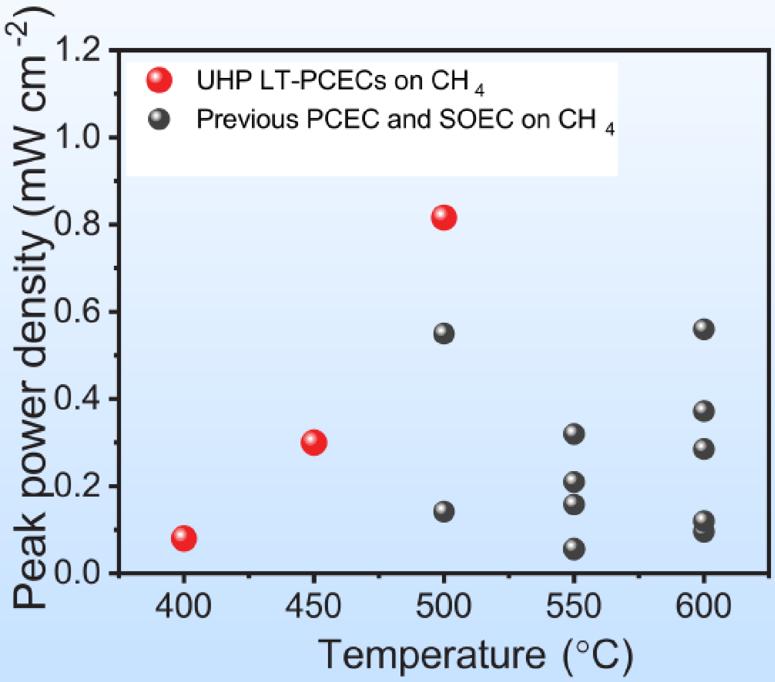
Advanced cathode materials for reducing electrode polarization resistance

Liu, F, Duan, C et al. Nature Energy 8.10 (2023): 1145-1157.

Progress and Current Status of Project

Task 4 – Reactor design, fabrication, and characterization.



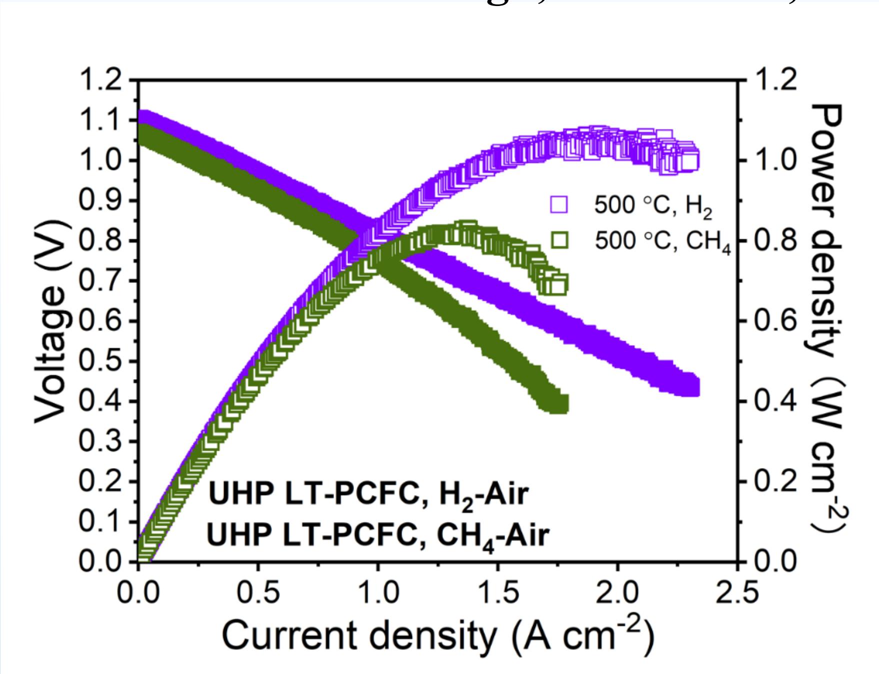


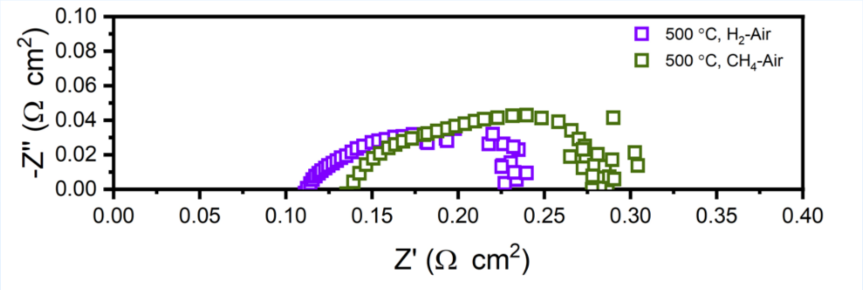
Methane-fueled fuel cell for power generation

Unpublished results

Progress and Current Status of Project

Task 4 – Reactor design, fabrication, and characterization.





Methane-fueled fuel cell for power generation

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Progress and Current Status of Project

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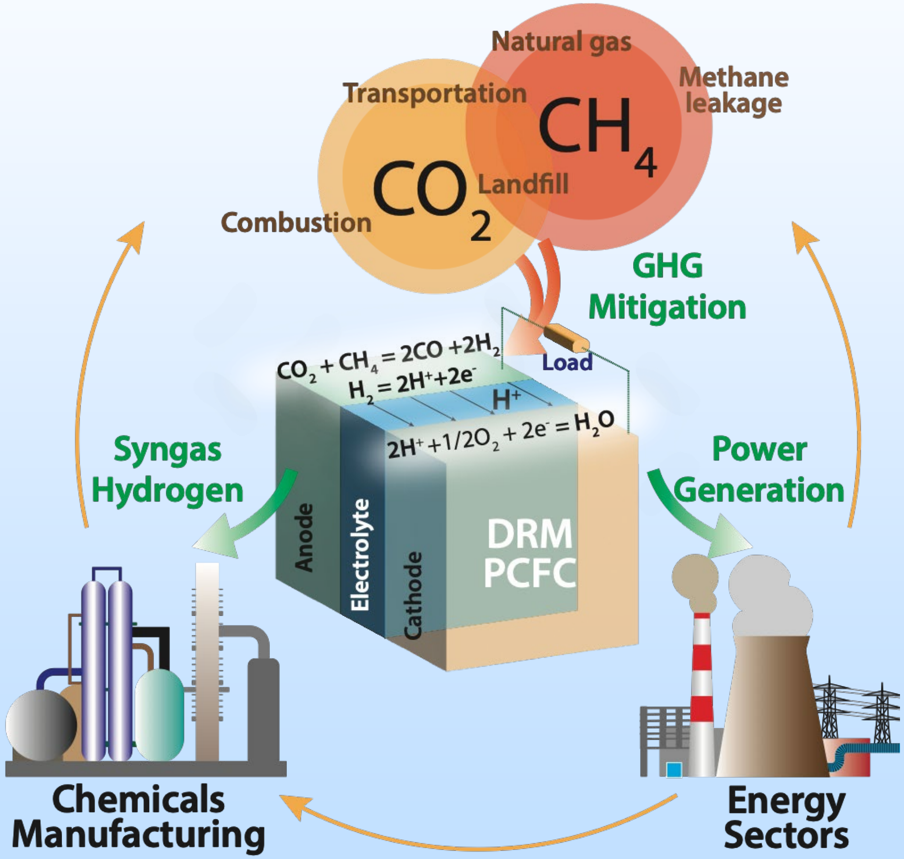
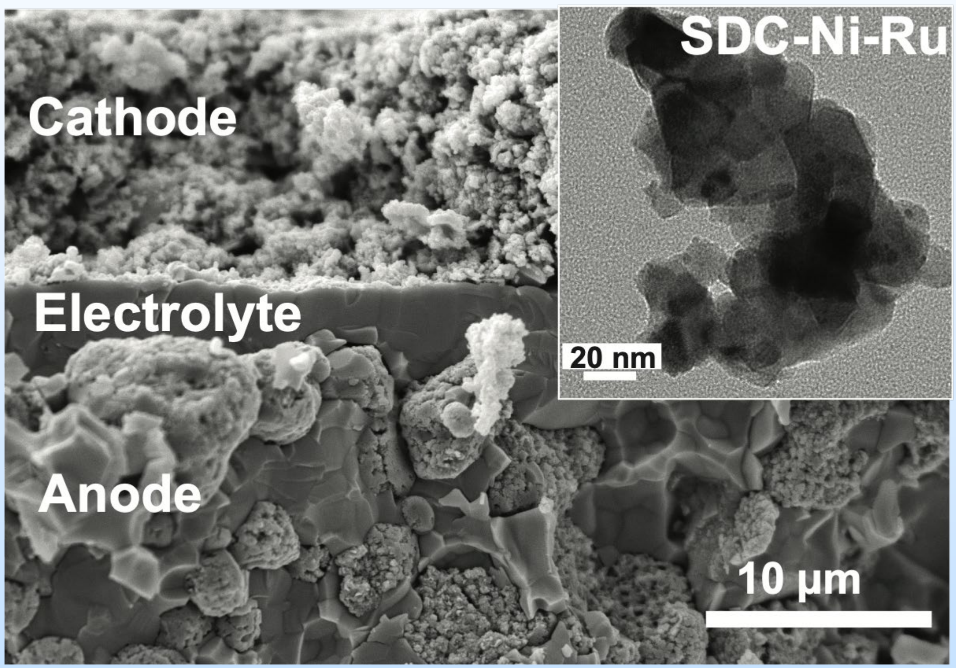
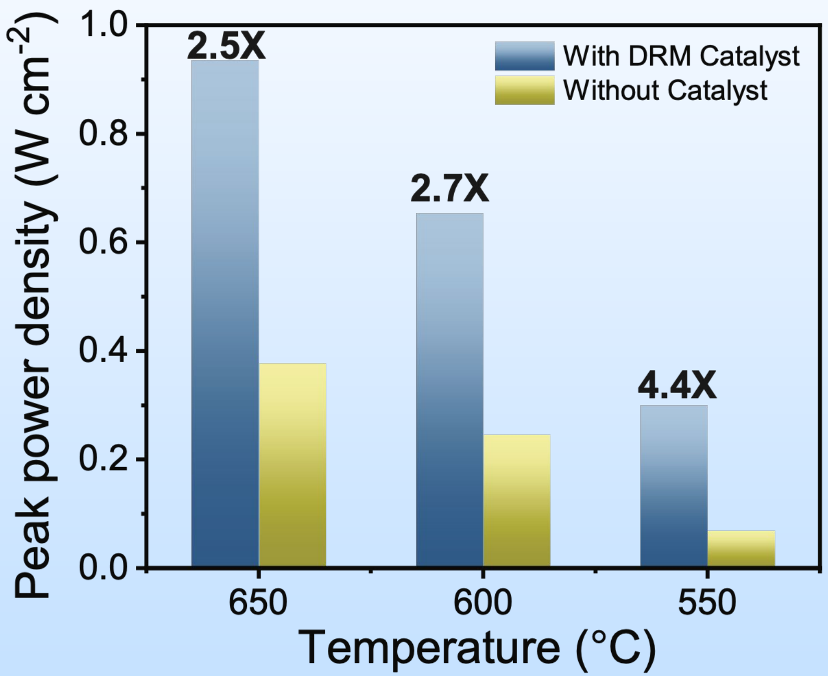


Ceramic electrochemical cells for mitigating emissions, syngas production, and power generation

Progress and Current Status of Project

Task 4 – Reactor design, fabrication, and characterization.





Ceramic electrochemical cells integrated with the dry reforming of methane catalysts improve performance

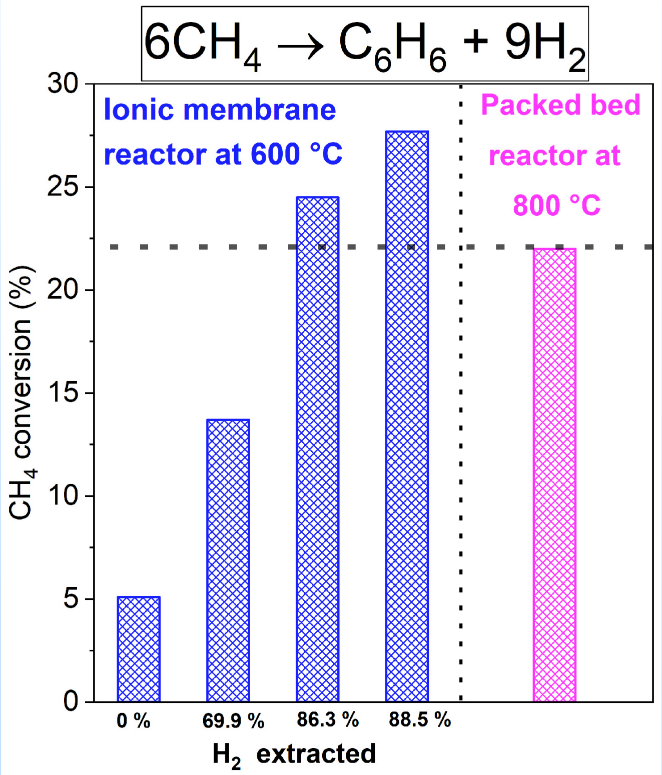
Progress and Current Status of Project

Task 4 – Reactor design, fabrication, and characterization.

Large-area tubular reactor manufacturing
Up to 200 cm^2

Progress and Current Status of Project

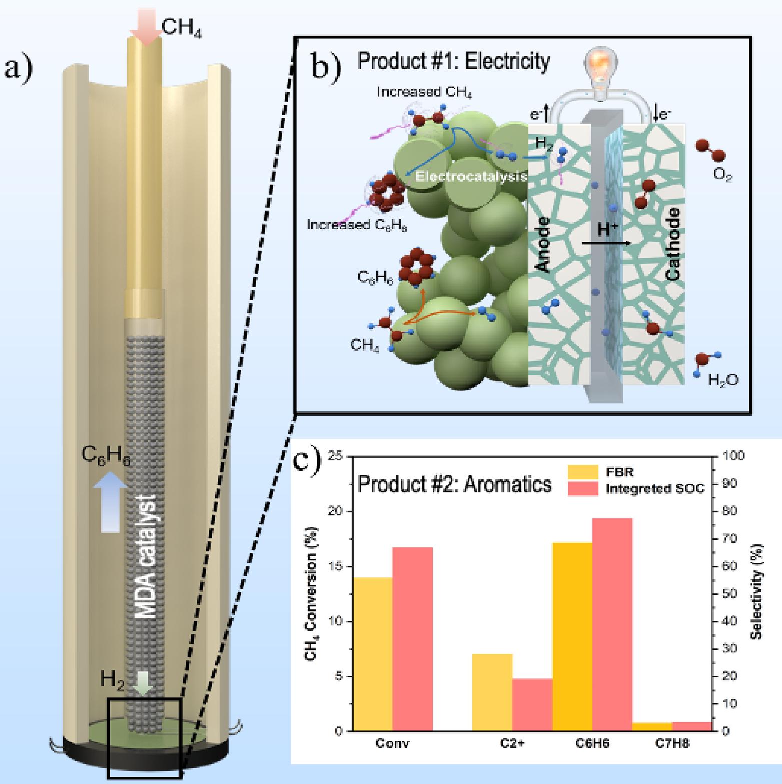
Task 5 – Demonstration of the process-intensified system

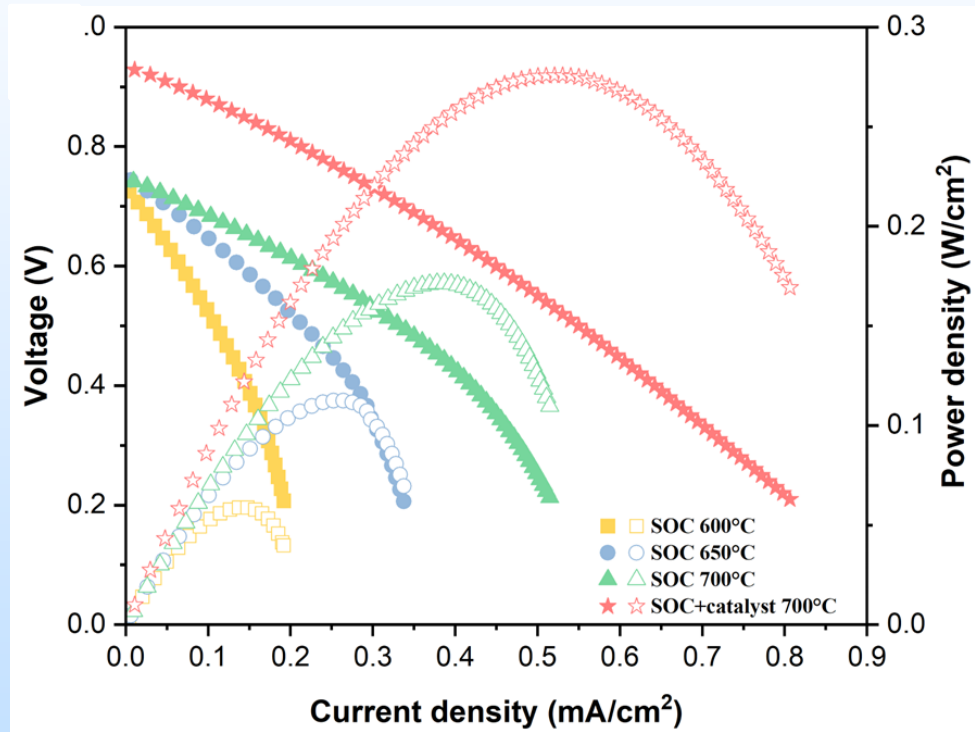


Reduced operating temperature can inhibit coking and improve durability

Progress and Current Status of Project

Task 5 – Demonstration of the process-intensified system





- Reduced operating temperature
- Enhanced conversion and selectivity to benzene
- Co-generation of power

Unpublished results

Plans for future testing/development/ commercialization (1-2 Slides)

- To achieve the TRL 6, the post-project work should be done include developing a large-scale PCEMR manufacturing process and prototype an industrially relevant system.

- Upon the accomplishment of this project, our team aim to secure additional funding from federal agencies and private foundations to bring the TRL to TRL 6.

- Additionally, we will also collaborate with ceramic membrane reactor manufacturers to produce the reactors in a large scale.

- Moreover, we will also work close with gas and oil industries to deploy the modular reactor, enabling to convert stranded natural gas onsite to high-value chemicals and electrical energy.

Outreach and Workforce Development Efforts or Achievements (If Applicable)

Workforce Development

- Support the training of 3 PhD students
- Help more than 10 undergraduate students to develop hands on research experience

Summary Slide

- The tri-metallic Pt-Bi/Mo/ZSM-5 improves both CH_4 conversion and selectivity to aromatics
- The ceramic electrochemical membrane reactors can generate power using natural gas.
- Tubular ceramic membrane reactors have been successfully fabricated.
- Preliminary demonstration of co-production of aromatics and power in the integrated reactor.
- The ceramic electrochemical membrane reactor enhances methane conversion and selectivity to aromatics, while generating power simultaneously.

cduan@ksu.edu, Materials Research Lab for Sustainable Energy

Acknowledgement

U.S. DEPARTMENT OF ENERGY
Fossil Energy and Carbon Management

DE-FE0032235

NATIONAL ENERGY TECHNOLOGY LABORATORY

Program Manager: Andrew E. Downs

The UNIVERSITY of OKLAHOMA

cduan@ksu.edu, Materials Research Lab for Sustainable Energy

Appendix

– These slides will not be discussed during the presentation but are mandatory.

Organization Chart

- Describe project team, organization, and participants.
  - Link organizations, if more than one, to general project efforts (i.e., materials development, design, systems analysis, pilot unit operation, management, risk/cost analysis, etc.).

- Please limit company specific information to that relevant to achieving project goals and objectives.

Organization Chart

Senior Personnel/Organization	Expertise	Roles and Responsibilities
Kansas State University Dr. Chuancheng Duan	Electrochemical membrane reactors; Electrocatalysis; Process intensification	Lead Tasks 1, 4, and 5. Project Management; PCEMRs development; System integration and testing.
University of Oklahoma Dr. Hanping Ding	Catalyst synthesis, characterizations, performance evaluation.	Lead Task 3 to deliver highly active and durable catalyst.
University of Oklahoma Dr. Pejman Kazempoor	Computational modeling to understand the degradation and operation, TEA, system design, and analysis	Lead Tasks 2, 6, and 7. Perform Computational analysis to guide the system design and process intensification, TEA, and LCA

Gantt Chart

Task name	Assigned Resources	Year 1	Year 2	Year 3
Task 1 – Project Management and Planning	KSU			
Task 2 – Establishing desired end states and identifying most suitable path from initial to end.	OU			
Task 3 – MDA catalysts development.	OU			
Task 4 – Fabricating and testing tubular PCEMRs.	KSU			
Task 5 – System integration and process intensification to realize direct conversion of natural gas.	KSU			
Task 6: Computational modeling of the proposed modular and process intensified system.	OU			
Task 7: Complete a comprehensive techno-economic and life cycle analyses of the natural gas conversion technology	OU			

Technical Approach/Project Scope

Project schedule

Milestone	Task/ Subtask	Milestone Title and Description	Planned Completion Date
M 1.1	Subtask 1.1	Project management plan	30 days
M 1.2	Subtask 1.2	Working with DOE and NETL to revise and finalize PMP	Q1
M 2.1	Task 2	Accomplish a comprehensive technology analysis plan (TAP) reviewed and confirmed by all project stakeholders	Q2
M3.1	Subtask 3.1	Achieve MDA conversion rate at 25% and selectivity towards aromatics >90% at 700 ^{o}C in the fixed-bed reactor mode.	Q2
M3.2	Subtask 3.2	Determine the elementary reaction steps of MDA and limiting step for designing an efficient catalyst.	Q3
M3.3	Subtask 3.3	Achieve >95% activity recovery after catalyst regeneration and overall <20% degradation rate on methane conversion in 20 h at 700 ^{o}C.	Q6
M4.1	Subtask 4.1	Fabricate novel tubular PCEMRs with a length of >10 cm and an active area of >50 cm^2.	Q6
M4.2	Subtask 4.2	Experimentally validated performance characteristics of the tubular PCEMRs. Achieve a methane conversion of >30% and a 50% increase in aromatics yield.	Q8
M5.1	Task 5	Demonstrate the modular and process intensified system.	Q10
M5.2	Subtask 5.2	Achieve >100 hours of testing using real natural gas as the feedstock.	Q12
M6.1	Task 6	Demonstrate the performance of the proposed reactor beyond the experimental points	Q9
M7.1	Subtask 7.1	Develop and report a comprehensive and validated performance model.	Q12
M7.2	Subtask 7.2	Develop and report a comprehensive and validated Economic analysis, including capital cost estimation and operation and maintenance costs.	Q11
M7.3	Subtask 7.3	Develop and report a comprehensive life cycle analysis for the proposed technology	Q12

Technical Approach/Project Scope

Project success criteria

Date	Go/No-Go Decision Point	Success Criteria
Q4	Tubular membrane reactors	Successfully fabricate novel tubular membrane reactors with a length of >10 cm and an active area of >50 cm^2.
Q12	Demonstrate the modular system and experimentally validate the performance	Achieve >30% methane conversion, >50% increase in aromatics yield, and >90% reduction in GHG emissions.

Project risks and mitigation strategies

Financial risks associated with securing next stage funding	We anticipate financing commercialization via global partnerships, replicating the KSU approach successfully implemented for natural gas conversion.
Technical risks associated with modeling	Model's ability to predict the overall system performance will be improved via empirical data collected during reactors tests.
The proposed efforts will be executed at two sites.	The team has collaborated on active or pending DOE projects. We have established successful collaborations.
Flammable gases	Lab safety notebooks and manuals have been established.