### Safety Moment

# Global Warming Making Spring Allergies Bloom Earlier

**RESEARCHERS SAY GLOBAL WARMING IS LEADING TO LARGER PLANTS AND EARLIER AND STRONGER POLLINATION** 

#### What You Can Do

Start early on allergy medication – trees may bud early, so don't wait to take medicine

Take antihistamines at night – their effectiveness peaks in the morning

Nasal washes are a natural alternative - follow proper water prep guidelines 385 plant species in Europe are blooming earlier than ever. In U.S. and Canada, ragweed season is up to 27 days longer

> Allergic rhinitis generates more than 12 million doctor visits each year.

35 million Americans are allergic to pollen and mold.

njhealth.org 1.877.CALL NJH (877.225.5654)

© National Jewish Health, 2013

## Common spring allergies

- Tree and grass pollen
- Mold spores

lational Jewish

Science Transforming Life®

Health

Dust mites & cockroaches
Animal dander



Π

## Annual meeting DE-FE0032005

Reversible Methane Electrochemical Reactor as an Efficient Energy Storage for Fossil Power Generation

Pejman Kazempoor, Ph.D (OU)

Chuancheng Duan, Ph.D. (KSU)

April 20, 2023

This presentation does not contain any proprietary, confidential, or otherwise restricted information



#### Sustainable and Alternative Energy Sources



#### **Carbon Management**



Sustainable Energy and Carbon Management Center



For more information, please contact Dr. Pejman Kazempoor (pkazempoor@ou.edu)

# Smart Production Through Digitization



Energy Storage and Management



Developing solutions that are locally appropriate; socially beneficial; economically and technically feasible; and environmentally responsible.



# AOI 3: Innovative Concepts & Technologies

"Substantial number of energy storage technologies are relatively **early-stage** in their development. ...The technologies need additional R&D to clarify their current state, understand their suitability for future advancement and integration, and to advance their maturity through R&D."

#### Reversible Methane Electrochemical Reactors for Fossil Energy Storage



#### Protonic ceramic electrochemical reactor

## **Project Objectives**

Conduct a comprehensive R&D program to demonstrate the suitability and future advancement and integration of reversible methane electrochemical reactors as an Efficient Energy Storage (EES) with fossil fuel power plants.

## Distinguish feature of the proposed technology

1- Direct Integration with fossil assets including fossil power plants and fossil-fuel industrial applications

2- PCERs exhibit high  $H_2S$  tolerance and coking tolerance

3- Reversible methane electrochemical cells display a high theoretical round-trip efficiency

4- Reduced operating temperatures enable hybridization with a broader range of waste heat sources



## Technology integration with existing or new fossil assets

**Indirect integration**: CO<sub>2</sub> is captured and separated through an intermediate system before entering the reversible PCER. CO2H2O CO2H2O

**Direct integration**: the flue gas enters the system without additional complex separation and purification processes to capture CO<sub>2</sub>, allowing significant cost reduction.



## **Define the Proposed Energy Storage Technology**

### **Systems Design Processes**

- 1. Characterize the initial state
- 2. Identify references to accomplish the general objective
- 3. Specify the proposed energy storage as the desire end states;
- 4. Define and consolidate the parameters and processes required to transform the initial energy storage technology into the desired end states
- 5. Assess the respective development or deployment status of the technology required for each function to yield technology needs.



<sup>2</sup> Interrelationships among the System Design Processes. NASA

[1] https://pragmaticarchitect.wordpress.com/2013/05/14/how-to-build-a-roadmap-define-end-state/ [2] https://www.nasa.gov/seh/2-fundamentals

## DOE Status and Targets for Reversible Solid Oxide Performance and Cost

- Stack cost target of \$225/kW
- System cost target of \$900/kW
- Less than 0.2% per 1,000 hours over an operating lifetime of 40,000 hours
- Efficiency of greater than 60% without carbon capture and storage

Metric	2018 Status	2020 Targets	2025/2030 Targets
System Cost (\$/kWe)	>12,000	6,000	900
System Degradation (%/1000 hrs)	1-1.5	0.5-1.0	>0.2
Durability (hr)	<2000	5000	8000
Fuel	Natural gas	Natural gas Simulated syngas	Natural gas Coal-derived syngas
Demonstration Scale	50 kWe – 200 kWe	200 kWe – 1 MWe	10-50 MWe

## Recent development of cell configuration to increase current density



Kobayashi, T., Kuroda, K., Jeong, S., Kwon, H., Zhu, C., Habazaki, H., & Aoki, Y. (2018). Analysis of the anode reaction of solid oxide electrolyzer cells with BaZr0. 4Ce0. 4Y0. 2O3-δ electrolytes and Sm0. 5Sr0. 5CoO3-δ anodes. Journal of The Electrochemical Society, 165(5), F342.

Choi, S., Davenport, T. C., & Haile, S. M. (2019). Protonic ceramic electrochemical cells for hydrogen production and electricity generation: exceptional reversibility, stability, and demonstrated faradaic efficiency. Energy & Environmental Science, 12(1), 206-215.

Huan, D., Shi, N., Zhang, L., Tan, W., Xie, Y., Wang, W., ... & Lu, Y. (2018). New, efficient, and reliable air electrode material for proton-conducting reversible solid oxide cells. ACS applied materials & interfaces, 10(2), 1761-1770.

Kim, J., Jun, A., Gwon, O., Yoo, S., Liu, M., Shin, J., ... & Kim, G. (2018). Hybrid-solid oxide electrolysis cell: A new strategy for efficient hydrogen production. Nano Energy, 44, 121-126.

Compositions of electrolyte (E) and cathode (C)*	Power density	Features	Year	Refs
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.2</sub> O <sub>3=δ</sub> (10 μm)	650 °C: 851 mW cm <sup>-2</sup>	Modification of $La_{0.5}Sr_{0.5}FeO_{3-6}$ with molybdenum	2021	31
C: La <sub>0.5</sub> Sr <sub>0.5</sub> Fe <sub>0.9</sub> Mo <sub>0.1</sub> O <sub>3-δ</sub>	700 °C: 1174 mW cm <sup>-2</sup>			
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.2</sub> O <sub>3-δ</sub> (15 μm)	600 °C: 486 mW cm <sup>-2</sup>	Modification of LaMnO3 with calcium	2021	32
C: La <sub>0.5</sub> Ca <sub>0.5</sub> MnO <sub>3-6</sub>	650 °C: 701 mW cm <sup>-2</sup>			
	700 °C: 1155 mW cm <sup>-2</sup>			
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.1</sub> Yb <sub>0.1</sub> O <sub>3-δ</sub> (25 μm)	500 °C: 270 mW cm <sup>-2</sup>	Development of a new triple-conducting electrode with improved	2021	33
C: Ba(Co <sub>0.4</sub> Fe <sub>0.4</sub> Zr <sub>0.1</sub> Y <sub>0.1</sub> ) <sub>0.95</sub> Ni <sub>0.05</sub> O <sub>3-6</sub>	550 °C: 450 mW cm <sup>-2</sup>	electrochemical activity and reduced thermal expansion		
	600 °C: 660 mW cm <sup>-2</sup>			
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.1</sub> Yb <sub>0.1</sub> O <sub>3=δ</sub> (24 μm)	600 °C: 311 mW cm <sup>-2</sup>	Ca-doping of La <sub>0.5</sub> Ba <sub>05</sub> Co <sub>0.8</sub> Fe <sub>0.2</sub> O <sub>3-5</sub> improves electrocatalytical	2021	34
C: La <sub>0.5</sub> (Ba <sub>0.75</sub> Ca <sub>0.25</sub> ) <sub>0.5</sub> Co <sub>0.8</sub> Fe <sub>0.2</sub> O <sub>3-6</sub>	650 °C: 489 mW cm <sup>-2</sup>	activity and reduces thermal expansion		
	700 °C: 716 mW cm <sup>-2</sup>			
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.1</sub> Yb <sub>0.1</sub> O <sub>3=δ</sub> (30 μm)	500 °C: 95 mW cm <sup>-2</sup>	Development of a new Ruddlesden-Popper electrode	2021	35
C: La0 25Sr2 75FeNiO7-8-BaCe0 7Zr0 1Y0 1Yb0 1O3-6	550 °C: 187 mW cm <sup>-2</sup>			
	600 °C: 334 mW cm <sup>-2</sup>			
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.1</sub> Yb <sub>0.1</sub> O <sub>3=6</sub> (14 $\mu$ m)	500 °C: 240 mW cm <sup>-2</sup>	Introduction of a porous $BaCe_{0.7}Zr_{0.1}Y_{0.1}Yb_{0.1}O_{3-\delta}$ interlayer	2021	36
C: La0 6Sr0 4Co0 2Fe0 8O3-8-BaCe0 7Zr0 1Y0 1Yb0 1O3-6	550 °C: 380 mW cm <sup>-2</sup>	between E and C		
	600 °C: 570 mW cm <sup>-2</sup>			
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.1</sub> Yb <sub>0.1</sub> O <sub>3=δ</sub> (25 μm)	500 °C: 188 mW cm <sup>-2</sup>	Tubular PCFC with a working electrode area of 2.3 cm <sup>2</sup>	2021	37
C: La <sub>0.6</sub> Sr <sub>0.4</sub> Co <sub>0.2</sub> Fe <sub>0.8</sub> O <sub>3.6</sub> BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.1</sub> Yb <sub>0.1</sub> O <sub>3.6</sub>	550 °C: 294 mW cm <sup>-2</sup>	·		
	600 °C: 465 mW cm <sup>-2</sup>			
E: BaCe <sub>0.6</sub> Zr <sub>0.2</sub> Y <sub>0.1</sub> Yb <sub>0.1</sub> O <sub>3-8</sub> (11 $\mu$ m)	500 °C: 420 mW cm <sup>-2</sup>	A Pd interlayer is introduced between E and C to improve the	2021	38
C: $PrBa_0 \leq Sr_0 \leq Co_1 \leq Fe_0 \leq O_{5+\delta}$	550 °C: 625 mW cm <sup>-2</sup>	interface electrochemical reactions		
	600 °C: 815 mW cm <sup>-2</sup>			
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.2</sub> O <sub>3-5</sub> (42 $\mu$ m)	600 °C: 316 mW cm <sup>-2</sup>	Pr-doping of a BaCe <sub>0.2</sub> Fe <sub>0.8</sub> O <sub>3</sub> electrode is performed to enhance	2021	39
C: BaCeo 2Feo 6Pro 2O2-5	650 °C: 447 mW cm <sup>-2</sup>	its electrochemical activity		
	700 °C: 562 mW cm <sup>-2</sup>			
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.2</sub> O <sub>3-5</sub> (15 $\mu$ m)	550 °C: 237 mW cm <sup>-2</sup>	A new triple-conducting electrode of $BaFe_{0.8}Ce_{0.1}Y_{0.1}O_{2.8}$ is	2021	40
C: BaFeo «Ceo 1 Yo 1O2.»	600 °C: 417 mW cm <sup>-2</sup>	proposed		
	650 °C: 530 mW cm <sup>-2</sup>	FF		
E: BaCe <sub>0.6</sub> Zr <sub>0.2</sub> Y <sub>0.1</sub> Yb <sub>0.1</sub> O <sub>7-5</sub> (15.7 $\mu$ m)	500 °C: 414 mW cm <sup>-2</sup>	This work confirms excellent electrochemical behavior of a	2021	41
C: PrBao sSro sCo1 sFeo sOs+s	600 °C: 685 mW cm <sup>-2</sup>	PrBao Sro Co1 SFeo OS+4 triple-conducting material		
ar 1 1 2 40,5 5 10,5 5 5 1,5 1 60,5 5 5 40	700 °C: 950 mW cm <sup>-2</sup>			
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.2</sub> O <sub>3-5</sub> (15 $\mu$ m)	600 °C: 545 mW cm <sup>-2</sup>	This work proposes new oxygen electrode with high	2022	42
C: $Sr_{2}Fe_{1} = MO_{0} = Sc_{0} = S$	650 °C: 965 mW cm <sup>-2</sup>	electrochemical activity and stability towards CO <sub>2</sub>		
5: 5:2: C1.5::00.250C0.250C0=0	700 °C: 1254 mW cm <sup>-2</sup>			
E: BaCe <sub>0.7</sub> Zr <sub>0.1</sub> Y <sub>0.2</sub> O <sub>3-6</sub> (8 $\mu$ m)	600 °C: 425 mW cm <sup>-2</sup>	A new combination of perovskite and lavered structured	2022	43
C: LaNio sFeo 4O2_s-Smo sSro sCoO2_s	650 °C: 728 mW cm <sup>-2</sup>	materials is proposed to be used as a cathode for PCFCs		
o. 10.10.01 e0.40.323 or10.3010.3000.320	$700 ^{\circ}\text{C}: 1427 \text{mW} \text{cm}^{-2}$	materials is proposed to be ased as a califord for 1 of os		
E: BaCeo «Zro »Yo »Ybo»O» « (15 µm)	500 °C: 262 mW cm <sup>-2</sup>	A complex modification (Ba-deficiency and Ni-doning) has been	2022	44
C: Bao os (Coo 4 Feo 4 Zro 1 Yo 1) o os Nio os O2-s	550 °C: 450 mW cm <sup>-2</sup>	proposed for improving functional properties of the state-of-the-		
0. 2.0.33( 0.0.4, 0.4.0.1, 0.1)0.33(0.0303=3	$600 ^{\circ}\text{C}; 672 \text{mW} \text{cm}^{-2}$	art triple-conducting BaCoo Feo 4Zro Yo 1Oa - material		
F: BaCee ZreaVerYherOe (157 µm)	$500 ^{\circ}\text{C} \cdot 171 \text{mW cm}^{-2}$	This work reports a successful application of	2022	45
C: SrCoo Feo Zro Yo Yo Oa BaCeo Zro Yo Ybo Oa	550 °C: 278 mW cm <sup>-2</sup>	SrCo <sub>2</sub> (Fe <sub>2</sub> 27 <sub>2</sub> , Y <sub>2</sub> , O <sub>2</sub> , cbased electrodes	2022	10
	$600 \text{ °C} 409 \text{ mW cm}^{-2}$			

\* Anode materials are not detailized in their compositions, since they (in oxidized forms) consist of NiO mixed with the electrolyte (E).

Cost Benchmarking of PCFC Versus SOFCs: (a) Cell and Balance-Of-Stack Component and (b) Total Stack Cost Distributions.





$$C_{cell} = \sum_{processes} (C_{mat} + C_{elec} + C_{labor} + C_{mach})$$

$$C_{mat}\left[\$ \ kWh^{-1}\right] = \frac{m_{cell} \ \left[kg \ cell^{-1}\right] \ast p_{mat}\left[\$ \ kg^{-1}\right]}{A_{cell} \left[cm^2 \ cell^{-1}\right] \ast p_{cell} \ \left[kW \ cm^{-2}\right]}$$

A significant power density improvement in PCFC or a lowercost sealant solution for the intermediate operation temperatures of PCFC are required in the future to close the gap of sealant cost with SOFC.

## Technical Targets (by DOE) and Achievements for High-Temperature Reversible Fuel Cells (Cell/Stack level)

#### SOFC RFC Technical Targets

Characteristic	Units	2020 Status	2030 Targets	Ultimate Targets
Cell Performance/ Roundtrip Electrical Efficiency at 0.5 A/cm2 FC; 1 A/cm <sup>2</sup> EL	%	80	80	85
Cell Durability/Degradation Rate <sup>,</sup>	%/1000 hr	<1.5	0.25	0.125
Stack Capital Cost (based on FC power output)	\$/kW	500	330	300
System				
System Roundtrip Efficiency	%	-	40	50
Roundtrip System Efficiency (includes thermal energy input)	%	37	60	70
Lifetime/Durability <sup>,</sup>	hr [Cycles]	10,000 <sup>7</sup> [unknown]	40,000 [1667]	80,000 [3333]
Levelized Cost of Storage	\$/kWh	1.11	0.20	0.1011
System Capital Cost by Power	\$/kW	-	\$1750	\$1250
System Capital Cost by Energy	\$/kWh	-	250	150



https://www.hydrogen.energy.gov/pdfs/review20/fc332\_wei\_2020\_o.pdf

Peterson, D. (2020), Reversible Fuel Cell Targets, DOE Hydrogen and Fuel Cells Program Record : 20001.

Choi, S., Davenport, T. C., & Haile, S. M. (2019). Protonic ceramic electrochemical cells for hydrogen production and electricity generation: exceptional reversibility, stability, and demonstrated faradaic efficiency. Energy & Environmental Science, 12(1), 206-215

Duan, C., Kee, R. J., Zhu, H., Karakaya, C., Chen, Y., Ricote, S., ... & O'Hayre, R. (2018). Highly durable, coking and sulfur tolerant, fuel-flexible protonic ceramic fuel cells. Nature, 557(7704), 217-222.

#### Previous Protonic ceramic electrochemical reactor for power generation and chemicals production





https://doi.org/10.1016/j.nanoen.2022.107722 л

Get rights and content 2

#### Abstract

Protonic ceramic <u>electrochemical cells</u> (PCECs) are solid-state <u>electrochemical devices</u> that employ proton-conducting oxides as electrolytes, which offer a promising approach for electrification of chemical manufacturing, including CO<sub>2</sub> reduction to produce valueadded chemicals (e.g., CO). The primary advantage of PCECs is their intermediate operating temperatures (300–600°C), which thermodynamically and kinetically favor the CO<sub>2</sub> reduction chemistry at the <u>negative electrode</u>. However, the conventional negative electrodes of PCECs, such as BaZr<sub>0.8-x</sub>Ce<sub>x</sub>Y<sub>0.2</sub>O<sub>3-6</sub>-Ni or BaZr<sub>0.8-x</sub>Ce<sub>x</sub>Y<sub>0.1</sub>Yb<sub>0.1</sub>O<sub>3-6</sub>-Ni, cannot reduce CO<sub>2</sub> to either CH<sub>4</sub> or CO with a selectivity of >99 %, leading to the

# Research Activity 1 at KSU: high-performance protonic ceramic fuel cells (PCFCs)



**Figure 1.**  $BaCe_{0.4}Zr_{0.4}Y_{0.1}Yb_{0.1}O_3$  electrolyte membrane conductivity of PCECs fabricated via SSS and SSRS.

**Figure 2.** SEM images and grain size of electrolyte membrane of PCECs fabricated via SSS and SSRS.

**Figure 3.** The Ultra-high-performance PCFC demonstrated at KSU exhibits the lowest Ohmic resistance.

### Highly conductive electrolyte membrane

# Research Activity 1 at KSU: high-performance protonic ceramic fuel cells (PCFCs)



Figure 1. Ultra-high-performance KSU Gen-2 PCFC recently demonstrated at KSU.

### Word record PCFC performances

#### Research Activity 1 at KSU: high-performance protonic ceramic fuel **Double SSS anode** cells



June

July-Aug

Sep-Oct

# Research Activity 1 at KSU: high-performance protonic ceramic fuel cells (PCFCs)





Highly active electrodes at intermediate operating temperatures

Reduced operating temperature favors CO<sub>2</sub> methanation

# Research Activity 1 at KSU: high-performance protonic ceramic fuel cells (PCFCs)



Durable PCFC performances at intermediate operating temperatures

Word record PCFC performances under methane

## **Research Activity 2** at KSU: CO<sub>2</sub> methanation catalysts



#### ACS APPLIED MATERIALS

#### acsami.org

Enhanced CO<sub>2</sub> Methanation Activity of Sm<sub>0.25</sub>Ce<sub>0.75</sub>O<sub>2.6</sub>–Ni by Modulating the Chelating Agents-to-Metal Cation Ratio and Tuning Metal–Support Interactions

Fan Liu, Yoo Sei Park, David Diercks, Pejman Kazempoor, and Chuancheng Duan\*

#### Cite This: ACS Appl. Mater. Interfaces 2022, 14, 13295–13304 🛛 🔇 Read Online

#### ACCESS Metrics & More Article Recommendations

ABSTRACT: Highly active and selective CO, methanation calapits are critical to CO<sub>2</sub> upgrading, synthetic, natural gas production, and CO<sub>2</sub> emission reduction. Wet impregnation is widely used to synthesize oxide-supported metallic nanoparticles as the calapitot for CO<sub>2</sub> methanation. However, as the reagents cannot be homogeneously mixed at an atomic level, it is challenging to modulate the microstructure, crystal structure, chemical composition, and electronic structure of calapits via wet impregnation. Herein, a scalable and straightforward catalyst fabrication approach has been designed and validated to produce  $Sma_{12}C_{22}mO_{22}$ -supported NI (SDC–NI) is abte CO<sub>2</sub> methanianion catalyst. By varying the chelating agents-to-total metal cations ratio (C/1 ratio) during the catalyst synthesis, we can eadily and simulaneously modulate the microstructure, metallic surface area, crystal structure, chemical composition, and electronic structure of SDC–Ni; Consequently fine-tuning the oxide-support interactions and CO<sub>2</sub> methanation activity. The devage and significantly improves CO<sub>2</sub> conversion at 250 °C. A CO<sub>2</sub>-oc-E(I, yield G



3 Supporting Information

Research Article

>73% has been achieved at 250 °C. Furthermore, a stable operation of 51500 hours has been demonstrated, and no degradation is observed. Extensive characterizations were performed to fundamentally understand how to tune and enhance CO<sub>2</sub> methanation activity of SDC–Ni by modulating the CI/ratio. The correlation of physical, demical, and cathylic properties of SDC–Ni with the CI/ratio is established and thoroughly daborated in this work. This study could be applied to tune the oxide—support interactions of various catalysts for enhancing the catalytic activity.

KEYWORDS: CO2 methanation, SDC-Ni, oxide-support interaction, structure-property relationship, in situ operando DRIFTS

13295

#### 1. INTRODUCTION

Converting CO2 and renewable H2 to CH4 can produce sustainable natural gas, reduce the reliance on fossil fuels, and decrease greenhouse gases emissions, leading to substantial economic and environmental benefits.1-4 CO2 methanation is thermodynamically favorable at 200-300 °C. However, CO2 molecules are very stable, and accordingly, high operating temperatures (>300 °C) are required to activate CO2 molecules and achieve practically valuable CH4 yield, necessitating the development of highly active catalysts for CO, conversion at <300 °C.56 However, CO, methanation at high operating temperatures consumes extensive energy and inevitably favors CO2-to-CO conversion, reduces the equilibrium CO<sub>2</sub> conversion, and decreases CH<sub>4</sub> yield and purity. Therefore, a CO<sub>2</sub> methanation catalyst that can attain a CH<sub>4</sub> selectivity of >99%, a CH4 yield of >70%, and a long operation stability at 250 °C is essential for economic renewable natural gas production. Despite enormous efforts that have been devoted to designing and synthesizing advanced CO2 methanation catalysts via novel approaches, such as noble metal-based catalysts,<sup>7-10</sup> metal-organic frameworks (MOF)-supported metallic nanoparticles,<sup>11,12</sup> and plasma treatment,<sup>13</sup>

© 2022 American Chemical Society

there are limited facial and scalable fabrication methods, which can readily fine-tune metal-support interactions to realize a  $CO_2$ -to- $CH_4$  yield of >70% with a long-term stable operation (>1000 hours) at 250 °C.

It has been recognized for a long time that synergistic interactions are exhibited between odds support and metallic nanoparticles. These interactions typically relate to the interactivative of metallic nanoparticles and oxide support, chemical compositions and electronic structure of both oxides and metalls nanoparticles, charge transfer between oxides and metals, and interfacial active area, which play essential roles in activating and converting CO<sub>2</sub>-lit-3 Modulating these metalsupport interactions is therefore a promising approach to improving CO<sub>2</sub>-conversion and Linning the CO<sub>2</sub> methanation

Received: December 9, 2021 Accepted: February 27, 2022 Published: March 9, 2022





## Research Activity 2 at KSU: CO<sub>2</sub> methanation catalysts



 $CO_2$  methanation catalyst synthesis approach by adjusting chelating agent/ion ratios (C/I)

## **Research Activity 3** at KSU: CO<sub>2</sub> conversion in PCECs



## **OU-Comprehensive Computational Modeling of Reversible Methane PCER**

 $CO + 3H_2 = CH_4 + H_2O (\Delta H_{298} = -206 \text{ kJ mol}^{-1}),$  $CO_2 + 4H_2 = CH_4 + 2H_2O (\Delta H_{298} = -165 \text{ kJ mol}^{-1}),$ 

Methane is formed through CO/CO2 hydrogenation.



PCEC voltage

2.0

0.20

Composite electrodes must deliver multiple physical processes: Gas, ion, and electron transport; catalysis; and electrochemistry

# Cell performance depends on the chemical potential of fuel and oxidizer and on internal losses



- Nernst potential equation based on the active species in each channel
- Cell operating voltage  $E_{op,f} = \delta * E_{op,i}$  $= \delta * [E_{Nernst,tot} - (\eta_{ohm} + \eta_{act} + \eta_{conc})]$

 $\eta_{ohm},\eta_{act}$  and  $\eta_{conc}$  are the ohmic, activation and concentration overpotentials

• Adjustment factor,δ

 $\delta = 0.00218 * T_{PEN} - 1.0683$ 

 $T_{PEN}$  is the cell operating temperature in Kelvin

## Model validation at different temperatures



#### **Comprehensive Techno-economic System Modeling of Reversible Methane PCER**



A Novel Hydrogen Economy based on Electrochemical Cells Using Water-Energy Nexus Framework

Proceedings of the ASME 2022 16th International Conference on Energy Sustainability ES2022 July 11-14, 2022, Virtual, Online



properties a selfantes a service value a efficience a terrar a structuristic.

### **Comprehensive LCA of Reversible Methane PCER**



In progress



Life Cycles Analysis of a novel integrated Hydrogen production system through water-energy nexus (Under Review)

## Levelized cost of hydrogen analysis

Taxes



# **Publications**

1-Jolaoso L.A, Asadi J, Duan C, Kazempoor P (2022). A novel green hydrogen production using water-energy nexus framework, Energy Conversion and Management, 276, 116344

2-Liu F; Fang L; Diercks D; Kazempoor P, Duan C, (2022) Rationally designed negative electrode for selective CO2-to-CO conversion in protonic ceramic electrochemical cells; Nano Energy, 102, 107722.

3-Liu F; Park Y; Diercks D; Kazempoor P, Duan C, (2022) Superior catalyst for synthetic natural gas production under mild condition, ACS Applied Materials & Interfaces 14 (11), 13295-13304.

4-Liu F, Diercks D, Kumar P, AbdulJabbar A, Gumeci C, Furuya Y, Dale N, Oku T, Usuda M, Kazempoor P, Fang L, Chen D, Duan C, Lower the operating temperature of protonic ceramic electrochemical cells to <450°C, Nature Energy (Under-review)

5- Liu F, Deng H, Ding H, Kazempoor P, Liu B, and Duan C, Processes-intensified protonic ceramic electrochemical cells for power generation, chemicals production, and greenhouse gas mitigation, Joule (Under-review)

6-Jolaoso L.A, Bello I.T, Ojelade O.A, Kazempoor P, A comprehensive review on Operational and scaling-up barriers of SOEC and mitigation strategies to boost H2 production, International Journal of Hydrogen Energy (under review)

7- Jolaoso L.A, Asadi J, Duan C, Kazempoor P (2022). Life cycles analysis of a novel integrated hydrogen production system through water-energy nexus, International Journal of Hydrogen Energy (Under Review )

Backup Slides

### Materials Research Laboratory for Sustainable Energy (MRLSE)

at Kansas State University

Chuanc Goo Assist

Tim Taylor Departmer Kansas

Please send me an email (cduan@ksu.edu) if you would like to join the group!

We have multiple PhD student and Postdoc open positions.

epresentative Publications

lick on figures below to see or download publications)













## **ELECTRODES AND BALANCED REACTIONS**

- Anode (steam channel)
- $4H_2O \rightarrow 8H^+ + 2O_2 + 8e^-$

Air (21%  $O_2$  and  $N_2$  balance) is added to this channel

- Cathode (fuel channel)
- CO<sub>2</sub> +8H<sup>+</sup> + 8e<sup>-</sup> → CH<sub>4</sub> +2H<sub>2</sub>O

Argon is feed to this channel to act as a sweep gas

**Overall reaction:** 

 $CO_2 + 4H_2O \rightarrow CH_4 + 2H_2O + 2O_2$ 

## **PCEC-GLOBAL CHEMICAL REACTION**

• The PCEC global chemical reaction for co-electrolysis of CO2 and H2O are:

- $CO_2 + H_2 \rightarrow CO + H_2O$ ,
- $CO + 3H_2 \rightarrow CH_4 + H_2O$ ,
- $CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O_1$

 $\Delta$ H=-41kJ/mol  $\Delta$ H=-206 kJ/mol

ΔH=-164 kJ/mol

## For Methanation-at the cathode

• 
$$CO_2 + 8H^+ 8e^- \Rightarrow CH_4 + 2H_2O$$
  
•  $E^0 = \frac{1}{8F} \left( \Delta_f G^0_{CO_2} - \Delta_f G^0_{CH_4} - 2 * \Delta_f G^0_{H_2O} \right)$   
•  $= \frac{1}{8*96487 \frac{C}{mol}} (-394.4 - (-50.9) - 2 * (-237.1)) \frac{kJ}{mol}$   
= 0.17 V



## Nernst and cell potential

At the anode

•  $E_{O2} = E_{O2}^0 - \frac{RT}{nF} ln \left( \frac{P_{H2O,an}^4}{P_{O2,an}^2 + P_{H2,an}^4} \right)$ 

At the cathode,

$$E_{CH4} = E_{CH4}^{0} - \frac{RT}{nF} ln \left( \frac{P_{CO2,ca} * P_{H2,ca}^{4}}{P_{CH4,ca} * P_{H2O,ca}^{2}} \right)$$

The open circuit voltage (OCV) is thereby given as:

- $E_{OCV} = \delta(E_{CH4} E_{O2})$
- $E_{Cell} = E_{OCV}$  + Overpotentials
- $\delta = f(T)$  is a balancing factor