Sustainable Conversion of Carbon Dioxide and Shale Gas to Green Acetic Acid via a Thermochemical Cyclic Redox Scheme

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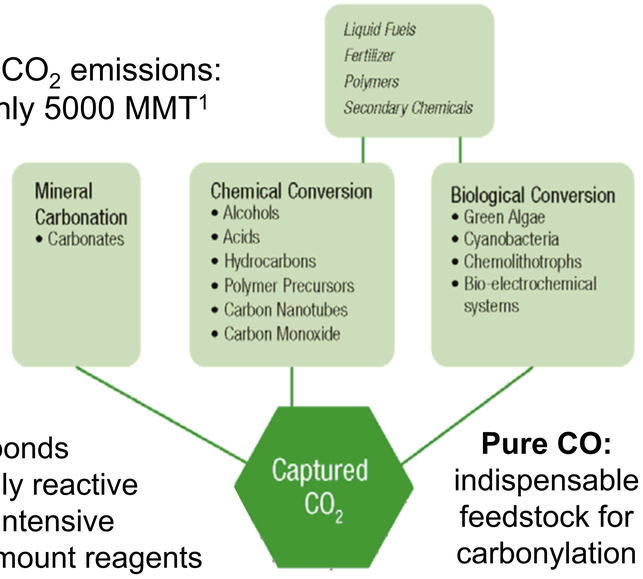
CO_2 Utilization

U.S. CO_2 emissions: roughly 5000 MMT[1]

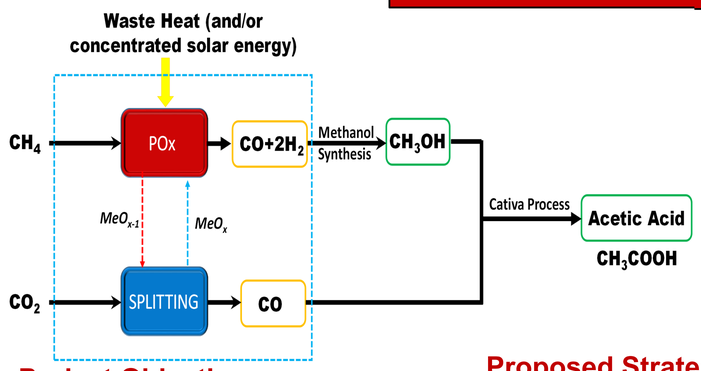


- Strong bonds
- Not highly reactive
- Energy-intensive
- Large amount reagents

Pure CO: indispensable feedstock for carbonylation

Efficient conversion of CO_2 to chemicals

Hybrid Redox Process (HRP)



U.S. Waste Heat Sources (Annual)		
Industry/ Furnace Type	Waste Heat @700° C (GJ)	CO_2 Converted (tonne/year)
Steel/EAF	36,547,000	6,180,000
Steel/BOP	14,300,000	2,260,000
Glass/Oxy-fuel	4,033,000	683,000

Project Objective

To develop a process for sustainable and cost-effective production of acetic acid, a critical building block for the plastic industry, from carbon dioxide and domestic shale gas resources

Proposed Strategy

To perform CO_2-splitting and methane partial oxidation (POx) in a synergistic two-step, thermochemical redox scheme via a hybrid redox process (HRP).

Potential Benefits

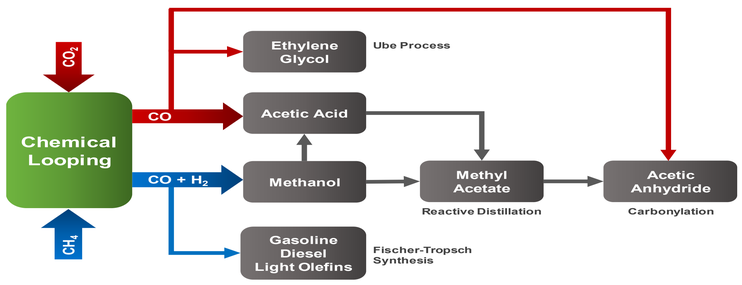
(i) Separate streams of methanol ready syngas and CO

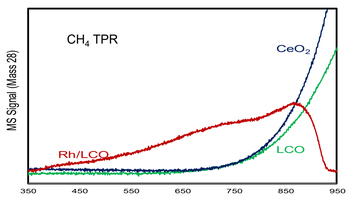
(ii) "low temperature" redox catalyst system for waste heat utilization

(iii) ability to produce other valuable chemicals, e.g. mono-ethylene glycol and acetic anhydride.

Key to Success: Effective redox catalyst particles

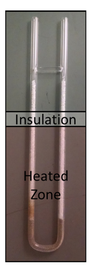
HRP Material Development

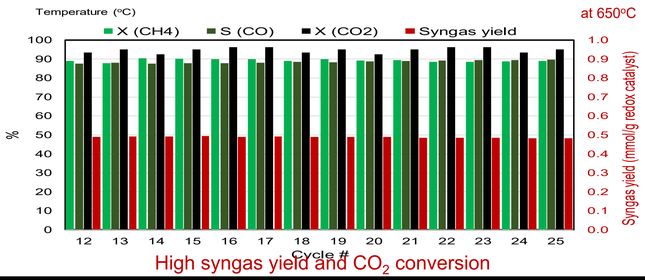




Presence of Rh on surface significantly reduces the apparent activation energy for surface reactions

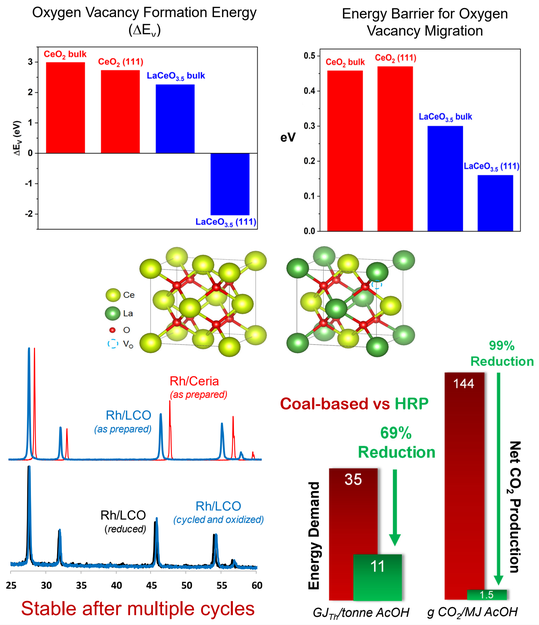
Sample	La 3d (%)	Ce 3d (%)	Rh 3d (%)
CeO_2		100.0	
LCO	64.1 *(50)*	35.9 *(50)*	
Rh/LCO	61.0 *(49.6)*	34.7 *(49.6)*	4.3 *(0.8)*





High syngas yield and CO_2 conversion

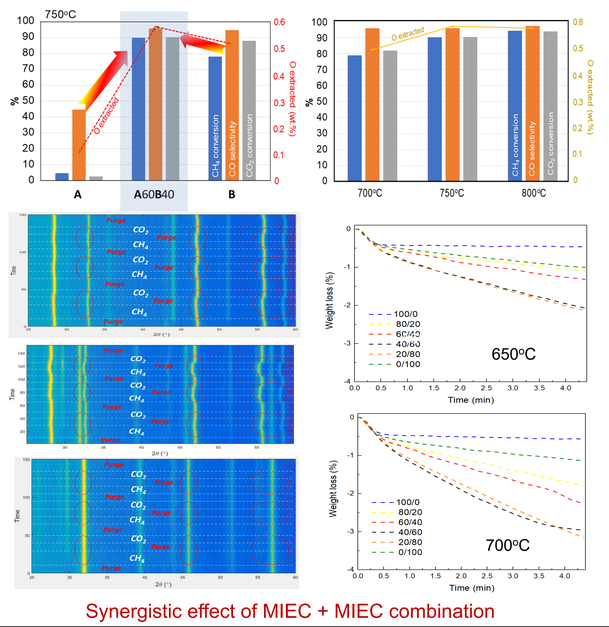
La-substituted Ceria Easier Oxygen Removal and Migration



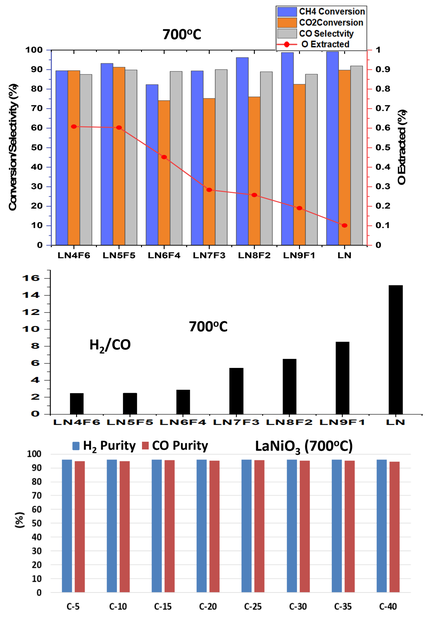
Stable after multiple cycles

PGM-free Redox Catalyst

MIEC (A) (CGCO) + MIEC (B) (LNF)



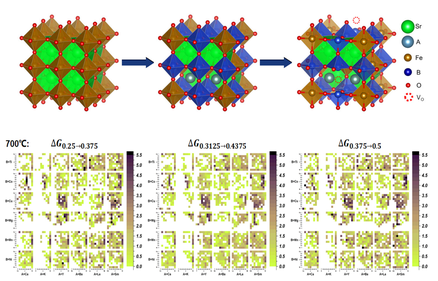
Standalone MIEC ($LaNi_xFe_{1-x}O_3$)

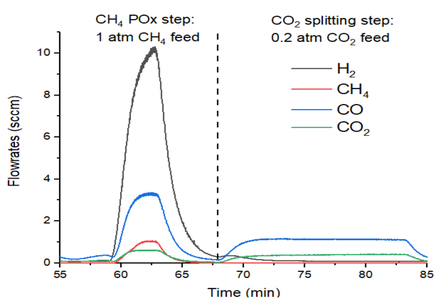


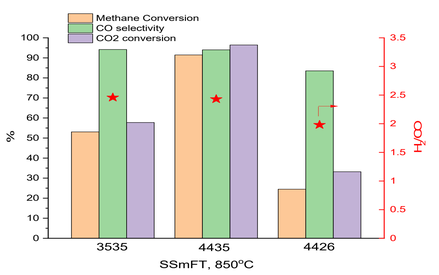
Synergistic effect of MIEC + MIEC combination

Redox Catalyst Optimization

DFT Guided Redox Materials Optimization

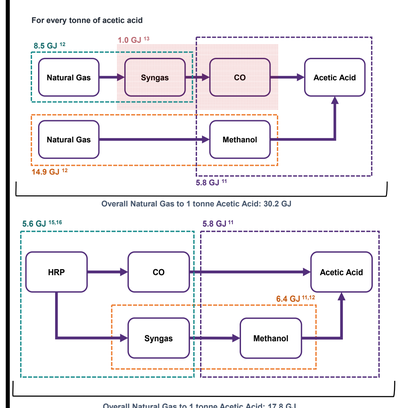


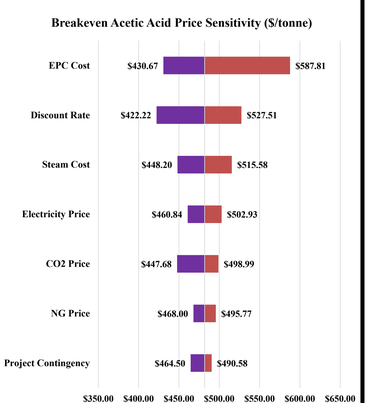


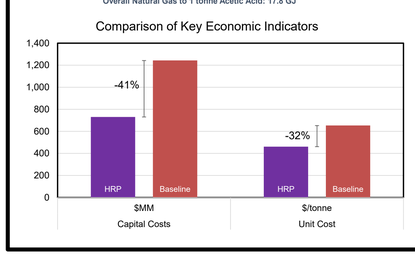


DFT guided selection of mixed-oxides with high activity and high lattice oxygen storage capacity.

Techno-Economic Analysis







41% capital savings with HRP.

32% reduction in cost per tonne of acetic acid vs. reference cost.

Task Name	Start	End	Resource	2019 Q1	Q2	Q3	Q4	2020 Q5	Q6	Q7	Q8	2021 Q9	Q10	Q11	Q12
Task 1 Project Managmant and Planding	2/1/2019	1/31/2022	NCSU/Susteon												
Milestone 1.1: PMP modification		2/28/2019	NCSU	◊											
Milestone 1.2: Project kickoff meeting		3/31/2019	NCSU/Susteon	◊											
Task 2.0: Redox material synthesis and characterizations	2/1/2019	6/30/2021	NCSU												
Subtask 2.1 Redox Material Synthesis	2/1/2019	6/30/2021	NCSU												
Subtask 2.2 Characterization of the Redox Materials	2/1/2019	11/31/2019	NCSU												
Milestone 2.1: Initial Redox material Screening		7/31/2019	NCSU		◊										
Milestone 2.2: Redox material down selection		10/15/2019	NCSU			◊									
Task 3.0: Redox Material Development	4/1/2019	6/30/2021	NCSU												
Subtask 3.1. Further characterization of the activity	4/1/2019	6/30/2021	NCSU												
Subtask 3.2. Optimization Strategy Development	7/1/2019	12/31/2020	NCSU												
Title: Milestone 3.1 Redox kinetics characterized		10/15/2019				◊									
Title: Milestone 3.2 Redox performance & stability		12/31/2019					◊								
Task 4.0: Techno-economic and Lifecycle Analysis	2/1/2019	12/31/2019	Susteon												
Subtask 4.1 Process model refinement and analysis	2/1/2019	12/31/2019	Susteon												
Subtask 4.2 Analysis of Alternatives Commercial Products	7/1/2019	12/31/2019	Susteon												
Milestone 4.1. Initial LCA TEA Report		12/31/2019	Susteon				◊								
Milestone 4.2 Product slate screening		10/15/2019	Susteon			◊									
Task 5.0: Redox Material: Long Term Stability	2/1/2020	6/30/2021	NCSU												
Subtask 5.1. Long term testing of the redox materials	2/1/2020	6/1/2021	NCSU												
Subtask 5.2 Empirical kinetic parameters analysis	2/1/2020	6/1/2021	NCSU												
Milestone 5.1 Reactor sizing		6/30/2020	NCSU					◊							
Milestone 5.2. Large lab-scale performance verification		12/31/2020	NCSU							◊					
Task 6.0: Techno-Economic and Life Cycle Analyses Update	2/1/2020	6/30/2021	Susteon												
Milestone 6.1 Reactor size/sensitivity		9/30/2020	Susteon						◊						
Milestone 6.2 TEA/LCA Update		12/31/2020	Susteon							◊					
Task 7.0: Redox Material : Economics Driven Optimizations	2/1/2021	12/31/2021	NCSU												
Subtask 7.1 Techno-economic Redox Catalyst Optimization	2/1/2021	12/31/2021	NCSU												
Subtask 7.2 Synthesis optimization for scale-up	2/1/2021	12/31/2021	NCSU												
Milestone 7.1 Optimized reactor Sizing		6/30/2021										◊			
Milestone 7.2 Scalable up material validation		12/31/2021													◊
Task 8.0: Development of detailed reactor and process	2/1/2021	12/31/2021	Susteon												
Milestone 8.1 commercialization road map		12/31/2021	Susteon												◊
Milestone 8.2 Final TEA and LCA report		4/30/2022	Susteon												→

Project Partners: Susteon, Linde