FROM CAPTURED CO₂ TO VALUE-ADDED CHEMICALS: A PHOTOCHEMICAL APPROACH

Project Number: FWP #34698

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> U.S. Department of Energy National Energy Technology Laboratory **Direct Air Capture Kickoff Meeting** February 24-25, 2021

Program Overview

- a. Funding (DOE and Cost Share)DOE: \$4.5M Cost Share: \$0
- b. Overall Project Performance Dates:
 Oct 1, 2020 Sep 20, 2023
- c. Project Participants

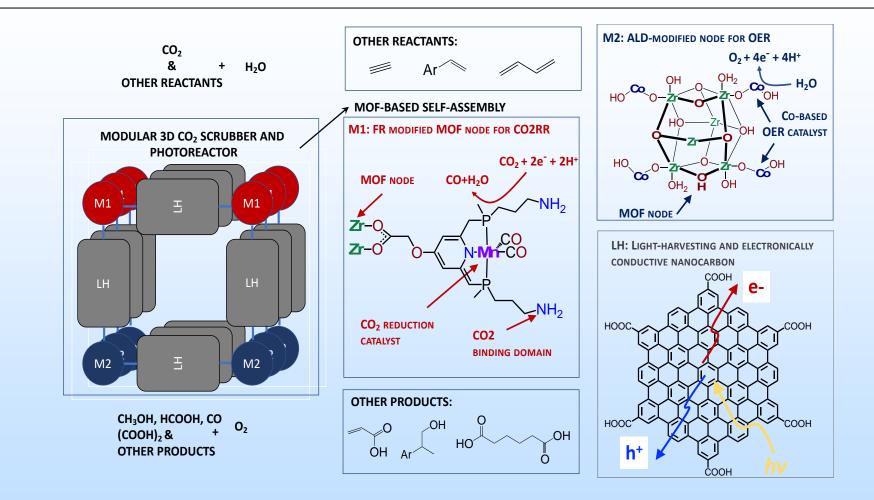
ANL: Chen, Glusac, Kaphan, Martinson, Mulfort, Tiede, Zapol

SLAC: Cordones-Hahn

d. Overall Project Objectives

Photoreactive capture that combines DAC of CO_2 with its direct conversion into fuels or value-added chemicals using visible light as an energy input.

Technology Background



Chromophores, catalysts and capture groups combined in MOFs. CO_2 release step avoided.

Technical Approach/Project Scope

- a. Experimental design and work plan
 Molecular Photoreactor Synthesis (Glusac, Martinson, Mulfort)
 DAC and Photocatalysis (Glusac, Kaphan and Zapol)
 Mechanisms (Chen, Cordones-Hahn, Glusac, Tiede and Zapol)
- b. Project schedule just provide key milestones; do not include a detailed Gantt chart
 - Year 1: synthesis of functionalized MOFs & catalyst discovery
 - Year 2: light-harvesting/charge separation studies & DAC screening
 - Year 3: proof-of-principle demonstration of photo-reactive capture
- c. Project success criteria
 - Demonstration of photo-reactive CO₂ capture
 - Mechanistic understanding of key steps of photoreactive capture
 - Identification of pathways toward improved systems

Team and Facilities

a. Photos of the team, including collaborators



Chen Cordones Glusac Kaphan Martinson Mulfort Tiede Zapol Hahn

b. Photos of facilities or specialized equipment

APS



SLAC

High-Throughput Research Lab

Laser Spectroscopy Labs Computer Clusters

Progress and Current Status of Project

 a. Description of the test equipment used/built in the project high throughput experimental setup (chemical and photochemical)

Femtosecond transient reflectance

b. Significant accomplishments and how they tie to the technology challenges

synthesis and scale-up of the first type of MOF crystals. This will enable future work with catalyst deposition.

c. Performance achieved so far when compared to project goals and how the performance relates to the economic and technical advantages

On track.

Opportunities for Collaboration

- a. Discuss how collaboration could have a synergistic effect on advancing the technologies described during the session
 Combining capture and conversion
 Use of sunlight as an energy input
- b. List potential areas of complementary work that others may contribute to this technology, including analysis, fabrication, modeling, engineering design, scale-up, etc.
 Engineering efforts to make a functional material.
 Scale-up from mg quantities.