U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Bioenergy Technologies Office 2023 Peer Review

Catalytic Upgrading

April 6, 2023

Sonia Hammache

Technology Manager

Reviewer Introductions

Name	Affiliation	Previous Peer Review Experience
Dr. Cory Phillips (Lead)	Director of Engineering Development, Air Company	2019, 2021
Dr. Qing Shao	Assistant Professor, University of Kentucky	2021
Dr. Chris Bradley	Program Manager, Catalysis Science Program DOE	2019
Dr. Xunhua Mo	Catalyst Development Scientist & Laboratory Supervisor, Johnson Matthey	New
Dr. Andrea Strzelec	Director for the Masters of Engineering in Engine Systems (MEES), University of Wisconsin-Madison	New

Catalytic Upgrading Agenda - Day 1

DAY 4 – Thursday, April 6, 2023					
8:00 AM	*10:00 AM*	120	*Registration, Breakfast, Plenary*	*All*	
10:00 AM	10:15 AM	15	Catalytic Upgrading Technology Area Introduction	BETO	Sonia Hammache
10:15 AM	10:50 AM	35	Overview of Chemical Catalysis for Bioenergy Consortium	NREL	Joshua Schaidle
10:50 AM	11:25 AM	35	Thermochemical Platform Analysis	NREL	Abhijit Dutta
11:25 AM	12:00 PM	35	Upgrading of C1 Building Blocks	NREL	Daniel Ruddy
12:00 PM	*1:00 PM*	*60*	*Lunch*	*All*	
1:00 PM	1:30 PM	30	ChemCatBio Data Hub	NREL	Frederick Baddour
1:30 PM	3:00 PM	90	Catalytic Upgrading of Biochemical Intermediates	NREL/PNNL/ORNL/LANL	Jeffrey Linger
3:00 PM	3:20 PM	20	*Break*	*All*	
3:20 PM	3:50 PM	30	Catalytic Upgrading of Pyrolysis Products for the Production of Sustainable Aviation Fuel	NREL	Mike Griffin
3:50 PM	4:20 PM	30	Low Pressure Hydrogenolysis Catalysts for Bioproduct Upgrading w/Visolis	PNNL/Visolis	Karthi Ramasamy
4:20 PM	*5:00 PM*	*40*	*Closed Door Comment Review Session*	*Reviewers*	

ChemCatBio Consortium

2021 Peer Review Feedback

2021 Review Panel findings:

- Successful consortium-based research
- Acceleration of the catalyst design cycle
- Systematic reduction of modeled MFSP through
  - Catalyst performance improvements
  - Process intensification
  - Production of high-value coproducts
- No specific gaps in technology or methodology within technology area
- Appropriate use of funding mechanisms for long-term support of National Labs

Consortia has critical importance using its unique strengths while funding industry partners to move toward commercialization

ChemCatBio produced world-class capabilities in enabling activities with far-reaching results. Real market impact: DFA linked industry partners with enabling programs to improve commercialization.

2021 Peer Review Feedback: Recommendations

1. Increase focus on ancillary technologies for producing high-value chemicals alongside core focus on producing high-volume fuels.
2. Expand scope of the Catalyst Deactivation Mitigation program to support process integration.
3. Develop strategic partnerships with catalyst manufacturers to facilitate scaling up next-generation materials.

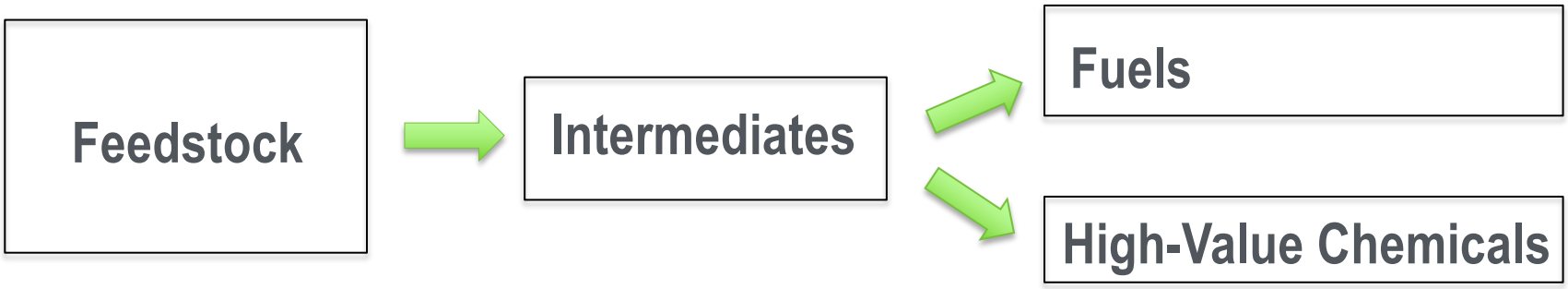
2021 Peer Review Feedback: Recommendation 1

1. High-value chemicals and materials have the clearest near-term path to market; accordingly, the program is encouraged to increase its focus on ancillary technologies for producing high-value chemicals alongside core technologies that focus on producing high-volume fuels.

Yes to high value chemicals in TEA

Focus on fuels

Bio-derived intermediates for fuel **or** high-value chemicals



2021 Peer Review Feedback: Recommendation 2

2. Catalyst stability remains problematic across the entire portfolio, and challenges presented by deactivation are likely to increase as technologies continue to mature and move toward process integration. Expanded access to ACSC and CCPC capabilities during the past decade has benefitted the entire portfolio. Along these lines, it would be prudent to expand the scope of the Catalyst Deactivation Mitigation program such that they can more effectively support efforts in process integration.

Continuing support for enabling projects

Limited to available funding

Enabling Capabilities

Advanced Catalyst Synthesis and Characterization
(NREL, ANL, ORNL)

Consortium for Computational Physics and Chemistry
(ORNL, NREL, PNNL, ANL, NETL)

Catalyst Deactivation Mitigation for Biomass Conversion
(PNNL)

2021 Peer Review Feedback: Recommendation 3

3. Eventual full-scale deployment of these catalytic technologies will require a transition to relatively large and formed catalyst pellets as opposed to the powders more common to bench-scale research. Mindful of this, the program is encouraged to develop strategic partnerships with catalyst manufacturers to begin the process of scaling up next-generation materials.

ChemCatBio FY23 *new 3-year cycle*

The following criteria should be addressed:

- By the end of the three-year cycle, produce the intended fuel i.e., sustainable aviation fuel, renewable diesel, or marine fuel. To date, most BETO-funded core projects have focused on optimization of the production of intermediate molecules.
- By the end of the three-year cycle projects are encouraged to use engineered catalyst forms relevant to the industrial application.
- Partnership with industry is highly recommended. Industry partnerships that can enable future deployment are desired (e.g., collaboration with a catalyst manufacturer to develop engineered catalysts.)

Relevant 2030 BETO Goals

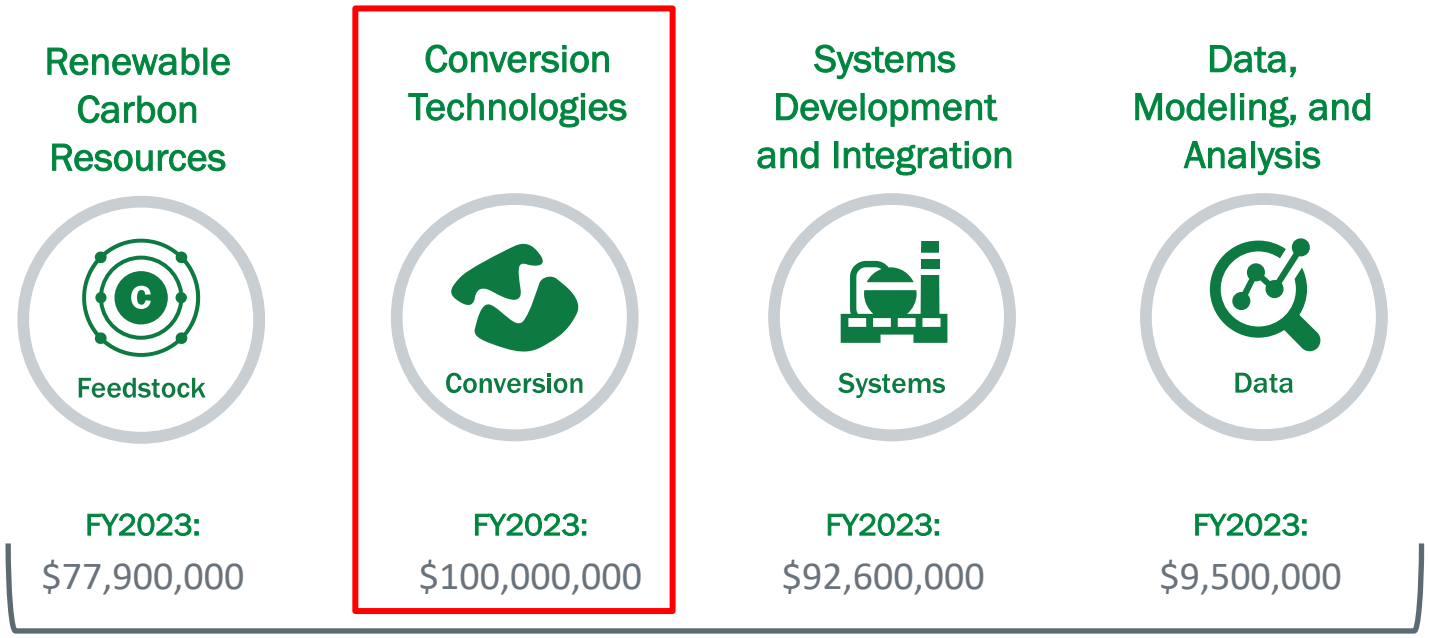
- **Support scale-up of sustainable aviation fuel (SAF) and other biofuels with >70% GHG emissions reduction**
- **Enable 10+ renewable chemicals and materials with >70% GHG emissions reduction**
- Enable 1+ cost-effective and recyclable bio-based plastic with >50% GHG emissions reduction

BETO Strategy: Catalyst Development

- Improve the selectivity to desired molecules, ideally in single-pass conversion to improve process carbon and energy efficiency.
- Assess the impacts of impurities present in bio-derived streams on catalyst performance. This defines the requirement to mitigate such impacts through clean-up or separations or by catalyst reformulation.
- Investigate catalyst deactivation mechanisms through joint computational and experimental approaches to improve catalyst formulation.
- Shorten the timeframe of technology development through engineered catalyst forms early in the research process.

BETO Program Areas

FY2023 Budget Authority = $280M



Budget Breakdown – Catalytic Upgrading

Type	FY22-FY23
ChemCatBio AOPs	$22MM
ChemCatBio Industry DFAs	(Phase I and II): $2.57MM
AOP	1.06MM
FOA Project	(all Pre-FY20): $1.927MM
TOTAL Session	$27.56MM

ChemCatBio Consortium Overview

Integrated and collaborative portfolio of catalytic technologies and enabling capabilities
New Cycle started in FY23

Core Technologies

Catalytic Upgrading of Biochemical
(NREL, PNNL, ORNL, LANL)

(NREL)

Upgrading of C2 Intermediates
(PNNL, ORNL)

Catalytic Fast Pyrolysis**
(NREL, PNNL)

Enabling Capabilities

Advanced Catalyst Synthesis and Characterization
(NREL, ANL, ORNL)

Consortium for Computational Physics and Chemistry
(ORNL, NREL, PNNL, ANL, NETL)

Catalyst Deactivation Mitigation for Biomass Conversion
(PNNL)

Industry Partnerships (Phase II Directed Funding)- completed in 2022

Opus12 (NREL)

Visolis (PNNL)

Sironix (LANL)*

Cross-Cutting Support

ChemCatBio Lead Team Support (NREL)

ChemCatBio DataHUB (NREL)

* Sironix is continuing under a no-cost extension.
** Changes in the CFP project

Changes in CFP Project in FY21

The project was not selected for scale up to meet program goal of demonstrating an industrially relevant process at $3/GGE targets due to the risks associated with adding hydrogen to the available equipment. The scope of work shifted to utilize prior work on zeolite catalyst for SAF production without requiring additional hydrogen

Project Review Criteria

You will be asked to provide a score for each of the three equally weighted criteria listed below:

1. Approach
2. Impact
3. Progress and Outcomes

The average scores from the review panel will be featured in the Final Peer Review Report.

Note the scores are from 1: Unsatisfactory to 5: Outstanding

Overall Impressions

You will then be asked to provide a written assessment of the project based on the above criteria. Please provide adequate rationale for each score. Please note that these comments will be featured in the Final Peer Review Report.

Housekeeping

Format:

- Each presentation is followed by 10 min Q&A
  First reviewers panel
  Then audience

- Umakanta Jena will be giving time checks
  (10 min, 5 min, 1 min remaining)

- Please do not take photos
  (ALL presentations will be posted publicly)

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Bioenergy Technologies Office 2023 Peer Review

Catalytic Upgrading

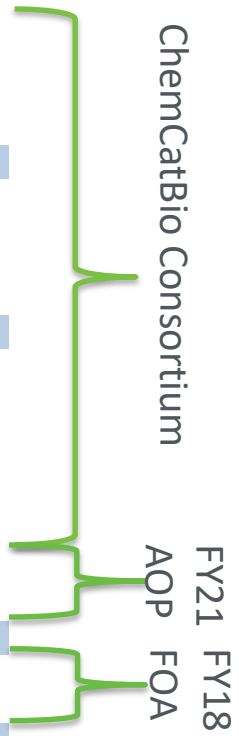
April 7, 2023

Sonia Hammache

Technology Manager

Catalytic Upgrading Agenda - Day 2

DAY 5 – Friday, April 7, 2023					
8:00 AM	*8:30 AM*	30	*Registration, Breakfast*	*All*	
8:30 AM	8:45 AM	15	Technology Area Daily Intro	BETO	Sonia Hammache
8:45 AM	9:15 AM	30	Upgrading of C2 Intermediates	ORNL	Andy Sutton
9:15 AM	9:45 AM	30	Upgrading of C2 Intermediates	PNNL	Robert Dagle
9:45 AM	10:15 AM	30	Catalytic Process Intensification of Bio-Renewable Surfactants Platform w/Sironix	LANL/Sironix	Claire Yang
10:15 AM	*10:30 AM*	15	*Break*	*All*	
10:30 AM	11:15 AM	45	Advanced Catalyst Synthesis and Characterization	NREL/ANL/ORNL	Susan Habas
11:15 AM	12:00 PM	45	Catalyst Deactivation Mitigation for Biomass Conversion	PNNL	Huamin Wang
12:00 PM	*1:00 PM*	60	*Lunch*	*All*	
1:00 PM	2:00 PM	60	Consortium for Computational Physics and Chemistry	ORNL	Jim Parks
2:00 PM	2:30 PM	30	Catalyst Development for Selective Electrochemical Reduction of CO2 to High-Value Chemical Precursors w/Opus-12	NREL/Opus 12	Frederick Baddour
2:30 PM	3:00 PM	30	Syngas Derived Mixed Olefin Oligomerization for Sustainable Aviation Fuel	PNNL	Karthi Ramasamy
3:00 PM	3:05 PM	5	*Break*	*All*	
3:05 PM	3:35 PM	30	Intensified Biogas Conversion to Value-Added Fuels and Chemicals	University of South Florida	John Kuhn
3:35 PM	4:00 PM	25	*Closed Door Comment Review Session*	*Reviewers*	



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ChemCatBio Consortium Enabling Capabilities

Enabling capabilities help shape CCB consortium through inter-laboratory communication and collaborations.

Core Technologies

- Catalytic Upgrading of Biochemical Intermediates (NREL, PNNL, ORNL, LANL)
- Upgrading of C1 Building Blocks (NREL)
- Upgrading of C2 Intermediates (PNNL, ORNL)
- Catalytic Fast Pyrolysis (NREL, PNNL)

Enabling Capabilities

- **Advanced Catalyst Synthesis and Characterization** (NREL, ANL, ORNL)
- **Consortium for Computational Physics and Chemistry** (ORNL, NREL, PNNL, ANL, NETL)
- **Catalyst Deactivation Mitigation for Biomass Conversion** (PNNL)

Industry Partnerships (Phase II Directed Funding)- completed in 2022

- **Opus12** (NREL)
- **Visolis** (PNNL)
- **Sironix** (LANL)*

Cross-Cutting Support

- **ChemCatBio Lead Team Support** (NREL)
- **ChemCatBio DataHUB** (NREL)

ChemCatBio Consortium: DFAs

Core Technologies

Catalytic Upgrading of Biochemical Intermediates (NREL, PNNL, ORNL, LANL)

Upgrading of C1 Building Blocks (NREL)

Upgrading of C2 Intermediates (PNNL, ORNL)

Catalytic Fast Pyrolysis (NREL, PNNL)

Enabling Capabilities

Advanced Catalyst Synthesis and Characterization (NREL, ANL, ORNL)

Consortium for Computational Physics and Chemistry (ORNL, NREL, PNNL, ANL, NETL)

Catalyst Deactivation Mitigation for Biomass Conversion (PNNL)

Industry Partnerships (Phase II Directed Funding)- completed in Sept 2022

Opus12 (NREL)

Visolis (PNNL)

Sironix (LANL)*

Cross-Cutting Support

ChemCatBio Lead Team Support (NREL)

ChemCatBio DataHUB (NREL)

* Sironix is continuing under a no-cost extension.

Directed Funding Awards (DFA)

CRADA Partnerships: Phase 2 Completed

Directed Funding Awards	Phase 1	Phase 2
Visolis @ PNNL: Low Pressure Hydrogenolysis Catalysts for Bioproduct Upgrading	• Catalyst identification and optimization • Catalyst stability 100 hrs.	• **Catalyst impurity tolerance** • **Extruded catalyst stability 500 hrs.**
Sironix @ LANL: Catalytic Process Intensification of Bio-Renewable Surfactants Platform	• Selective reduction & furan coupling catalysts • Optimize catalyst for scale up	• **Alternative coupling catalysts for new tail options** • **Develop and test catalysts for furan-tail coupling approaches**
Twelve @ NREL: Catalyst Development for Selective Electrochemical Reduction of CO_2 to High-value Chemical Precursors	• Cathode catalyst development • Reactor integration and catalytic evaluation	• **Scale up of cathode catalyst**

VISOLIS
CARBON NEGATIVE MATERIALS

SIRONIX
RENEWABLES

twelve

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Additional Projects from FOA and AOPs

- FY18 BioEnergy Engineering for Products Synthesis (BEEPS) - USF

Topic Area 1 - ChemCatBio collaborations aimed at tackling fundamental challenges in catalysis - catalyst characterization, catalyst development and R&D for producing engineering-relevant/technical catalysts. CCB National Laboratory partner required.

- Syngas Derived Mixed Olefin Oligomerization for Sustainable Aviation Fuel- Pacific Northwest National Laboratory (PNNL).

Lab Call 2022. AOI 3a: Sustainable Aviation, Diesel and Marine Fuels R&D:

Produce sufficient quantities of neat fuel (e.g. >250mL) to complete relevant testing protocols. Testing should, at a minimum, include Tier α and β properties for SAF and ASTM D975 for diesel and marine (or alternately ISO 8217 for marine)

Some Successes

- DFAs completed with positive appraisals from the industrial partners:

"… exploring these effects would have been difficult if not for the support of ChemCatBio…" Twelve/NREL

"*…..is providing invaluable technical development, resources, and expertise to solve one of our biggest technical challenges toward commercialization*" Sironix/LANL

"…..accelerated the low-pressure hydrogenolysis catalyst discovery and the process development cycle." Visolis/PNNL

- Industry led CRADAs furthering CFP process development and promoting commercial readiness (CRADAs – so Exxon, Johnson Matthey)
- Increased industry interest for the many pathways developed within ChemCatBio and AOP projects.
- Publications and patents: More than 140 publications and 29 patents and issues patents

Progress – FOAs and MSRDC: $6.76MM

2021 FOA: Topic area 5a Renewable Natural Gas (R&D)

- University of Virginia: Biogas Methanation via Advanced Ni Catalysts

2022 FOA: Topic Area 3 Robust Catalytic Processes

- University of Alabama: Sustainable Aviation Fuels from Biomass Derived Ethanol
- University of Kentucky: Robust Engineered Catalysts for the Conversion of Algae and Waste Oleaginous Biomass Feedstocks to Fuel-like Hydrocarbons via Decarboxylation/Decarbonylation (deCOx)

The MSI STEM Research & Development Consortium (MSRDC)

Focus Area 3: Accelerating catalyst development for biofuel production

- University of New Mexico: Improving Catalyst Stability and Durability for Conversion of Biomass Derived Feedstocks
- University of Maryland Baltimore County: Simulating Olefin Adsorption in Hierarchical Zeolites with Acid Sites

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