The Chemical Catalysis for Bioenergy Consortium: Enabling Production of Biofuels and Bioproducts through Catalysis

Josh Schaidle
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Catalysis Challenges are Pervasive in Biomass Conversion

**Challenges due to Biomass Composition**
- High oxygen content → new reactions
- Diverse chemical functionalities → competing rxns
- High water content → Degradation of cat. supports
- Impurities (S, N, alkali metals, Cl, etc.) → Poisoning
- Multiple states and compositions (solid, liquid, or gas)
- Complex, heterogeneous mixture → difficult to model

**Key Catalytic Bioenergy Processes**
- Lignin Deconstruction and Upgrading
- Catalytic Upgrading of Biological Intermediates
- Synthesis Gas Upgrading
- Catalytic Fast Pyrolysis
- Catalytic Hydroprocessing
- Catalytic Upgrading of Aqueous Waste Streams

*Catalyst costs can represent up to 10% of the selling price of biofuel*
Introducing the Chemical Catalysis for Bioenergy Consortium

ChemCatBio is a national lab led R&D consortium dedicated to identifying and overcoming catalysis challenges for biomass conversion processes

- **Our mission** is to accelerate the development of catalysts and related technologies for the commercialization of biomass-derived fuels and chemicals by leveraging unique US DOE national lab capabilities
- **Our team** is comprised of over 100 researchers from seven different national labs

*Advanced Synthesis and Characterization*  *Modeling and Interactive Tools*  *Multi-Scale Evaluation*
Our Approach

Establish an integrated and collaborative portfolio of catalytic technologies and enabling capabilities

Foundational Science

Advanced Synthesis and Characterization

Hydrotalcites

Theory

Bench-scale reactions

Product analysis

Applied Engineering

Catalyst Cost Estimation

Catalyst Scaling and Pilot-Scale Testing

Energy Materials Network

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ABLC Next 2017
**Market Opportunity:**
Increasing Demand for Premium Gasoline

**Technology Opportunity:**
Production of High-Octane Synthetic Alkylate from Biomass-Derived Dimethyl Ether

**Catalysis Challenge:**
Reactivate and reincorporate light alkane products (isobutane) into the chain growth mechanism, thereby maximizing C$_{5+}$ yield

→ Metal-modified HBEA
Syngas Upgrading: Catalyst Advancements

**Active Site**
Identified Cu(I) as the active site for i-C\textsubscript{4} dehydrogenation using *in-operando* X-ray Absorption Spectroscopy

**Reaction Mechanism**
Calculated energetics for 2-step mechanism over Cu(I) active site

**Performance Evaluation**
Demonstrated C\textsubscript{4} reincorporation

![Reaction coordinate diagram](image)

Outcomes:
- Reduced modeled fuel production cost by >$1/gal since 2015
- Identified promising bimetallic formulations for improved performance

C. Farberow, et al., *ACS Catalysis* 7 (2017) 3662

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ABLC Next 2017
Market Opportunity:
Renewable Fuel Standard Mandates for Advanced Biofuels

Advanced Biofuel Market Size: $7B - $15B per year

Technology Opportunity:
Woody Biomass Conversion to Gasoline and Diesel Blendstocks through Catalytic Fast Pyrolysis

Catalysis Challenge:
Improve carbon yields and extend catalyst lifetime

→ Leverage a fixed-bed system with co-fed H₂ operating at near atmospheric pressure over non-zeolite catalysts

Source: EPA, DOE Billion Ton Study


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Catalytic Fast Pyrolysis: Catalyst Advancements

**Surface Chemistry**
Determined role of acidic and metallic sites for CFP using advanced characterization.

**Deactivation Mechanism**
Identified deactivation mechanism using *in-situ* spectroscopy.

**Performance Evaluation**
Demonstrated improved oil yields for CFP and catalyst regenerability.

**Outcomes:**
- Reduced modeled fuel production cost by $0.85/gal since 2016
- Enhanced deoxygenation by tuning metal-acid bifunctionality

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M. Griffin, et al., *ACS Catalysis* 6 (2016) 2715
Catalytic Upgrading of Biochemical Intermediates: Market, Opportunity, and Challenge

Market Opportunity:
Biomass-Derived Oxygenates as Platform Chemicals

Technology Opportunity:
Hybrid Biological-Catalytic Route for Production of 1,4-Butanediol through Succinic Acid

Catalysis Challenge:
Enhance catalyst selectivity to 1,4-BDO and stability under acidic aqueous conditions
→ Bimetallic formulations

D. Vardon, et al., ACS Catalysis 7 (2017) 6207

Process operates under corrosive conditions:
- 170-190°C
- 100-120 bar H₂
- 5wt% succinic acid in water

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Catalytic Upgrading of Biochemical Intermediates: Catalyst Advancements

**Composition and Morphology**
Validated co-location of Ru and Sn using high-resolution scanning transmission electron microscopy

**Catalyst Stability**
Computationally determined bimetallic catalyst stability

**Performance Evaluation**
Converted corn stover-derived succinic acid to 1,4-BDO in a flow system

Outcomes:
- Identified a Ru-Sn bimetallic catalyst that achieved 71% yield to 1,4-BDO
- Developed computational models to predict stability of bimetallic catalysts

D. Vardon, et al., *ACS Catalysis* 7 (2017) 6207
ChemCatBio is releasing a free-of-charge catalyst cost estimation tool

The CCM tool enables:

- Meaningful **cost comparison** for pre-commercial catalysts at bulk scale
- Identification of **major cost drivers** to guide further research
- **Sensitivity/risk analysis** to aid commercialization of new catalysts and processes
- An assessment of the **value proposition** of advanced catalysts early in development

Due for release in 2018 as a downloadable spreadsheet and companion web app
Catalyst Cost Model Development: Approach

**Raw materials from grams to tons**

\[ \text{Ni(acac)}_2 + 0.5 \text{ TOP} \xrightarrow{\Delta \text{ solv.}} \text{Ni Nanocatalyst} \]

- Parameterized scale-up templates
- Up-to-date material pricing and industry standard scaling relationships
- Rapid and accurate early-stage catalyst cost estimation

**From Laboratory Steps to Unit Ops**

- Dissolution: 20-100°C
- Impregnation: 20-100°C
- Drying: 200-200°C
- Heat treatment: 200-700°C
- Pre-treatment: 200-400°C

**Materials and Prices**

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<th>Quantity (Lb)</th>
<th>Price ($/Lb)</th>
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</table>

**Ni(acac)₂ + 0.5 TOP solv.**

- Ni nanoparticles

**ChemCatBio**

- Chemical Catalysis for Bioenergy

**Energy Materials Network**

- U.S. Department of Energy
Analysis with the CCM tool enables an early assessment of the value proposition of a catalyst.

Catalyst performance metrics (e.g., lifetime, yields, regenerability) can be normalized by cost.

Expands early-stage catalyst design criteria to include production cost.
Announcements and Engagement Opportunities

• Awarded **$4.3M in Directed Funding Assistance** in September for industry to leverage ChemCatBio capabilities to overcome technical challenges in catalyst development and evaluation
  – 9 projects selected with 8 different industry partners
  – Gevo, Visolis, Vertimass, Lanzatech, ALD Nanosolutions, Johnson Matthey, Opus-12, and Sironix Renewables

• Seeking members for our **Industry Advisory Board**
  – Role: Guide the consortium toward industry-relevant R&D, provide a business perspective, and identify knowledge gaps
  – If interested, please contact us at Contact@ChemCatBio.org

• Organizing a **ChemCatBio Symposium at the 255th ACS National Meeting** in New Orleans on March 20th and 21st
  – Abstracts due Friday October 20th
  – Hosted in the Division of Catalysis Science and Technology (CATL)
Acknowledgements

For more information, please visit our website at ChemCatBio.org or email us directly at Contact@ChemCatBio.org
The Chemical Catalysis for Bioenergy Consortium:
Enabling Production of Biofuels and Bioproducts through Catalysis

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