CATALCHEM-E Project Descriptions

Catalytic Application Testing for Accelerated Learning Chemistries via High-throughput Experimentation and Modeling Efficiently

University of Wisconsin-Madison – Madison, WI

AI-Driven Design of Industrial Fixed Bed Reactor Catalysts for Production of Renewable Fuels and Chemicals from Oxygenated Feedstocks (AI-FIXCAT) - $2,835,000

The University of Wisconsin-Madison will develop catalysts to convert ethanol into higher-value alcohol for fuels and specialty chemicals. The project will combine AI models with automated laboratory tools and industrial-scale catalyst testing. The team will also explore integrating the technology into laboratory information management systems, making the catalyst design workflow accessible to a wide range of commercial entities.

Ames National Laboratory – Ames, IA

Autonomous High Throughput Experimentation to Accelerate Chemical Manufacturing (A-TEAM) - $2,520,000

Ames National Laboratory will deliver precious-metal-lean catalysts for specific hydrocarbon processing reactions, cutting energy use and boosting domestic manufacturing competitiveness. The project's collaborative workflow uses advanced AI models coupled with robotic synthesis platforms to rapidly explore new catalyst concepts. The workflow ensures industrial relevance through multiscale validation, from atomistic simulations to pilot-scale reactor testing.

North Carolina State University – Raleigh, NC

Human-AI-Robot Teaming to Accelerate Heterogeneous Redox Catalyst Discovery with a Self-Driving Lab - $2,992,500

North Carolina State University aims to discover catalysts for the conversion of biomass and other waste liquids into hydrogen-rich syngas, a critical industrial feedstock for fuels and chemicals. This platform distinguishes itself by integrating several cutting-edge innovations. These include AI for self-driving labs that learn from physics and employ intelligent optimization, automated synthesis, proxy screening methods, as well as transport modeling. These elements will collectively ensure new catalysts can be industrially scaled.

National Laboratory of the Rockies – Golden, CO

SYNTH-ON: An Autonomous Synthetic Framework to Power the Refinery of Tomorrow - $2,835,000

The National Laboratory of the Rockies plans to accelerate catalyst discovery using an AI-enabled automated workflow featuring high-throughput flow synthesis. This system will develop catalysts ten times faster, producing thousands of samples daily and scaling to enable kilogram-scale production. Initially, it will validate catalysts for the reverse water-gas shift reaction, then explore new materials to convert simple carbon molecules into valuable chemicals, reducing import reliance.

University of Connecticut – Storrs, CT

REACT: Revolutionary Enhancements in AI-Guided Catalyst Transformations - $2,916,450

The University of Connecticut's REACT project will develop an AI-powered workflow to discover electrocatalysts for directly converting methane gas into alcohols, which are crucial for producing fuels and chemicals. The team's "design-make-test-learn" workflow will use uncertainty-aware models with high-throughput experimentation to identify promising catalysts, which will then be validated in commercial-scale membrane electrode assemblies.

Pacific Northwest National Laboratory – Richland, WA

Trinity AI Platform Integrating Digital, High Throughput, and Scale-Up for Inverse Catalyst Development - $2,722,500

Catalyst development is often a slow process because findings from small laboratory tests do not always translate reliably to larger, engineered devices. Pacific Northwest National Laboratory's Trinity AI Platform (TAP) project will develop an automated, promotion-gated workflow where only the most promising catalyst candidates are advanced to more demanding, industrially relevant tests. The team will use this workflow to discover new electrocatalysts that convert waste carbon dioxide into ethanol. Promising catalysts will be validated directly in engineered electrodes, ensuring their relevance for industrial applications.

Idaho National Laboratory – Idaho Falls, ID

KINETIC: Knowledge Integration and Next-Generation Experiments to Transform Industrial Catalysis - $2,992,500

The Idaho National Laboratory's CATALYST project will develop catalysts to convert hydrocarbon resources into high-value chemicals and fuels. The project will combine robotic high-throughput synthesis with advanced transient testing methods to learn how catalysts behave dynamically at the microscopic level. Understanding how the catalyst's surface changes over time enables more adaptable chemical manufacturing.

University of Rochester – Rochester, NY

Catalyst Acceleration and Testing via AI and Language to Yield Scalable Transformations (CATALYST) - $2,992,500

The University of Rochester aims to accelerate catalyst deployment for the conversion of carbon dioxide to methanol and ethanol by developing a unique AI-enabled workflow. This project will use large language models to represent catalysts with text of synthesis procedures and reaction conditions. If successful, this approach will enable rapid language-driven discovery of new materials.

Argonne National Laboratory – Lemont, IL

Accelerated Catalyst Design Foundry - $2,771,100

Argonne National Laboratory will develop new catalysts to convert waste carbon feedstock into chemical feedstocks and energy carriers. The project aims to establish a comprehensive catalysis data library to curate experimental and computational data, enabling AI-driven predictions for catalyst design. By utilizing the latest advances in AI, high-throughput experimentation, and self-driving labs, the project aims to transform U.S. chemical manufacturing.

Lawrence Berkeley National Laboratory – Berkeley, CA

PANDORA: Platform Acceleration for Novel-catalyst Discovery and Optimization with Reactor-arrays and AI/ML - $2,835,000

Lawerence Berkeley National Laboratory will develop atomically tailored catalysts for the conversion of carbon dioxide into industrial commodity chemicals. The project team will develop advanced AI models with high-throughput reactor arrays and new surface chemistry investigation strategies. This approach addresses the bottlenecks in scaling catalyst production from initial gram-scale research to kilogram-scale manufacturing.

Oxylus Energy – Branford, CT

Project SPRINT-EC: Syngas Production via Rapid Inverse-design Network for Tailored Electrochemical Catalysts - $2,955,391

Oxylus Energy will develop an AI-accelerated workflow to discover electrocatalysts for the conversion of carbon dioxide to methanol. The project will use machine learning models that learn from many experiments simultaneously, from rapid initial screens all the way through testing in commercial electrolyzers to predict which catalysts will perform best at scale.

P2 Science, Inc. – Woodbridge, CT

HEAT FACTORY: Highly Energetic Advanced Turpentine Fuels Accessed with Catalytic Transformations Optimized Robotically - $2,834,879

P2 Science aims to dramatically speed up the discovery of catalysts for converting plant-based feedstocks, such as oils and resins from pine trees and citrus waste, into high-performance liquid fuels. The project will combine advanced robotics with machine learning in an automated system to rapidly test thousands of catalyst candidates. This approach will allow the team to identify catalysts that perform under milder, more efficient conditions, enabling the production of fuels compatible with existing engines, including in aviation.