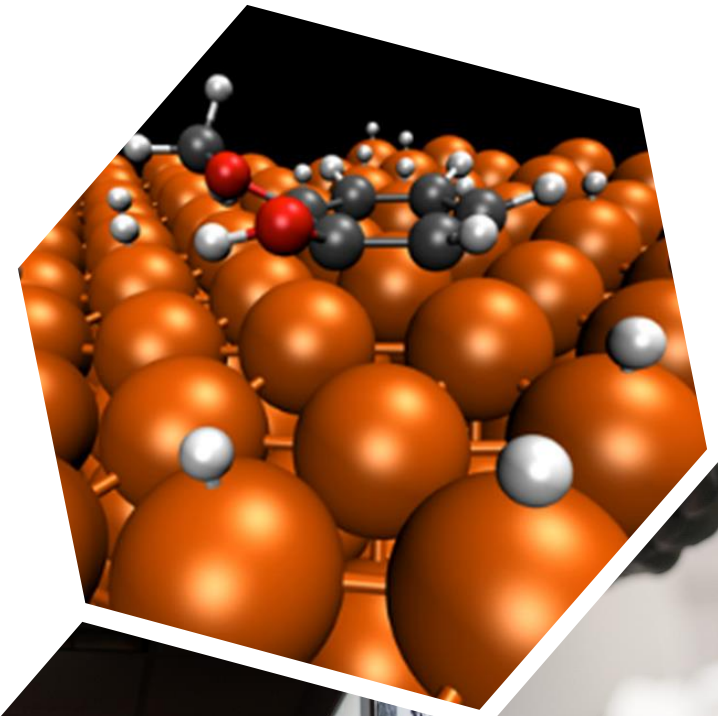
ChemCatBio
Chemical Catalysis for Bioenergy



ChemCatBio DataHub

WBS: 2.6.2.500

U.S. Department of Energy (DOE)
Bioenergy Technologies Office (BETO)
2019 Project Peer Review

Carrie Farberow

March 4th, 2019

U.S. DEPARTMENT OF ENERGY | Office of ENERGY EFFICIENCY & RENEWABLE ENERGY
BIOENERGY TECHNOLOGIES OFFICE

ChemCatBio Foundation

Integrated and collaborative portfolio of catalytic technologies and enabling capabilities

Catalytic Technologies

- **Catalytic Upgrading of Biochemical Intermediates** (NREL, PNNL, ORNL, LANL, NREL*)
- **Catalytic Upgrading of Indirect Liquefaction Intermediates** (NREL, PNNL, ORNL)
- **Catalytic Fast Pyrolysis** (NREL, PNNL)
- **Electrocatalytic and Thermocatalytic CO_2 Utilization** (NREL, ORNL*)

*FY19 Seed Project

Enabling Capabilities

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

Industry Partnerships (Directed Funding)

- **Gevo** (NREL)
- **ALD Nano/JM** (NREL)
- **Vertimass** (ORNL)
- **Opus12**(NREL)
- **Visolis** (PNNL)
- **Lanzatech** (PNNL) - Fuel
- **Gevo** (LANL)
- **Lanzatech** (PNNL) - TPA
- **Sironix** (LANL)

Cross-Cutting Support

ChemCatBio Lead Team Support (NREL)

ChemCatBio DataHUB (NREL)

Goal Statement and Outcomes

Goal

Enable **ChemCatBio** and the **bioenergy industry** to **accelerate** the **catalyst** and **process development** cycle by establishing the DataHub for:

1. **Centralized** and **secure** data **storage, sharing, and analysis**
2. Development and application of publicly available advanced analytics tools that provide **predictive capabilities** for catalyst R&D

Outcomes

- Data repository for **easy** and **fast storage and sharing** of data **amongst project teams** and, as desired, with the **public** for **knowledge dissemination**
- **Customized plug-ins** and **data analysis tools** to **increase research efficiency**
- **Integrated catalyst design engine** that accelerates the catalyst development process by **optimizing for predicted performance and material cost**

Relevance to Bioenergy Industry

- **Pathway-independent tools** developed **reduce** the **time and cost** to develop active, selective, low-cost and durable **real-world catalysts** to produce **desired end-products from biomass and waste resources**

Quad Chart Overview

Timeline

- Project start date: 10/1/2017
- Project end date: 9/30/2020
- Percent complete: 50%

	Total Costs Pre FY17**	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
DOE Funded	$0	$0	$200k	$400k

Barriers addressed

- Ct-F – Increasing the yield from catalytic processes
- Ct-G – Decreasing the time and cost to develop novel industrially relevant catalysts

Objective

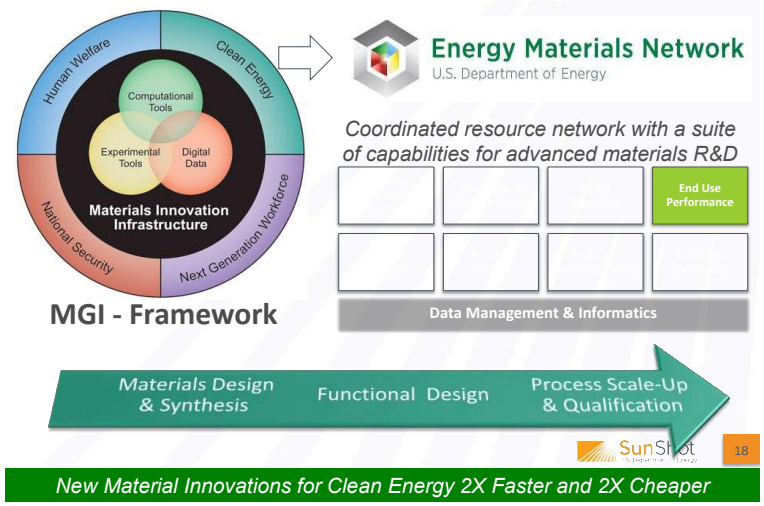
Develop and provide access to **accelerated data storage, sharing, and advanced analytics tools** to **reduce** the **time** and **cost** to **develop catalysts** for the production of desired end-products from biomass and waste resources.

End of Project Goal

Produce a **data repository** alongside **customized plug-ins and data tools** that are **accessible** to all ChemCatBio project teams and industry partners, including completion of the infrastructure of an **integrated catalyst design engine** that simultaneously **considers predicted performance and catalyst material cost** to accelerate the catalyst design cycle.

Overview: The ChemCatBio DataHub

In support of the Materials Genome Initiative, each DOE EMN consortium is tasked with providing an accessible, searchable data resource.

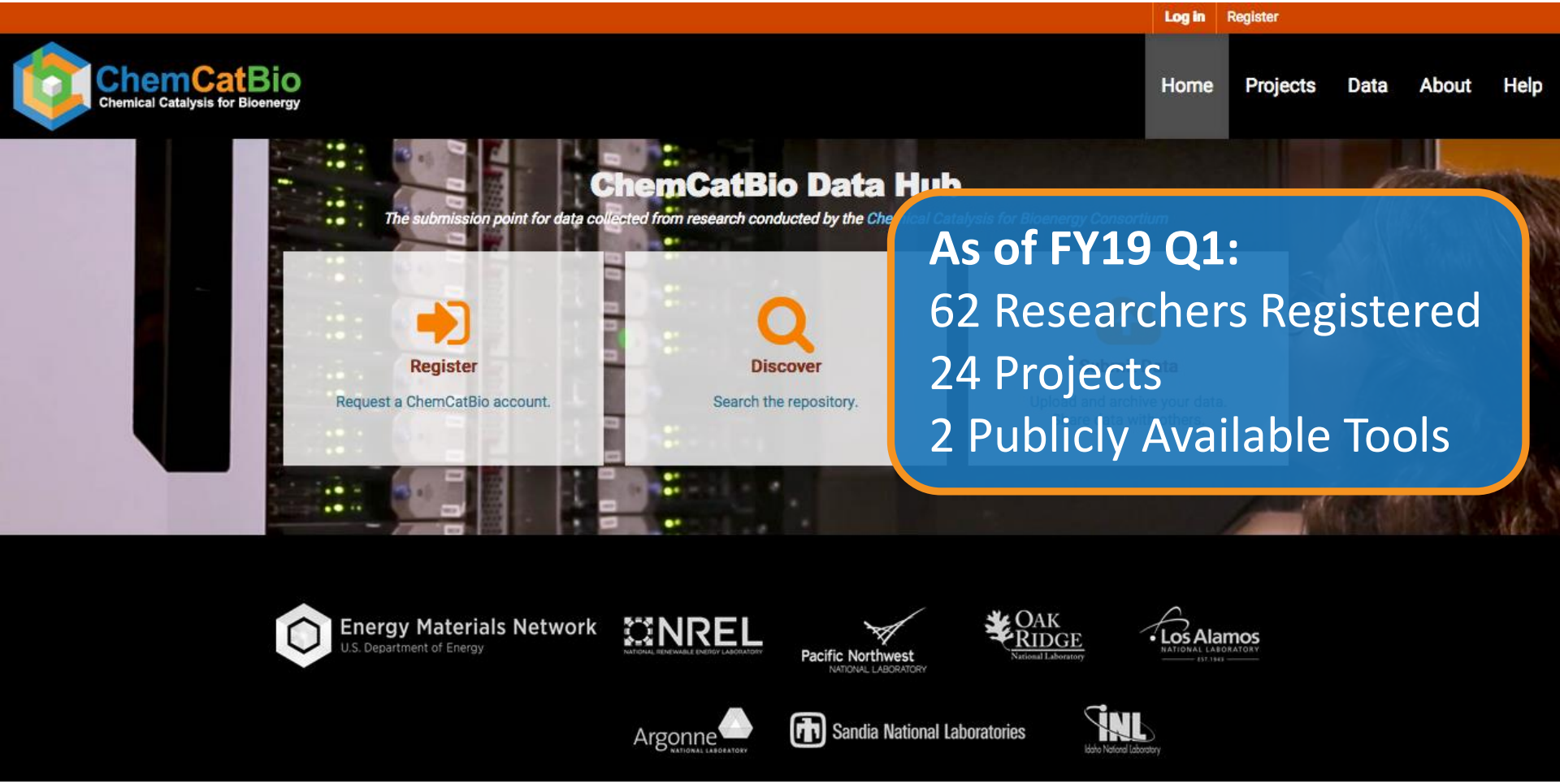


Key Project Outcomes

- Provides a **secure** project **space for storing and sharing project data**
  - ➢ *Outcome: Faster, less burdensome cross-institution collaboration*
- Enables **controlled public accessibility** of selected datasets
  - ➢ *Outcome: Distribution of knowledge and reduction in research redundancy*
- Facilitates development of and access to **advanced data analysis tools**
  - ➢ *Outcome: Application of state-of-the-art predictive approaches that accelerate catalyst R&D*

Overview: The ChemCatBio DataHub

The ChemCatBio DataHub is publically accessible at *datahub.chemcatbio.org*

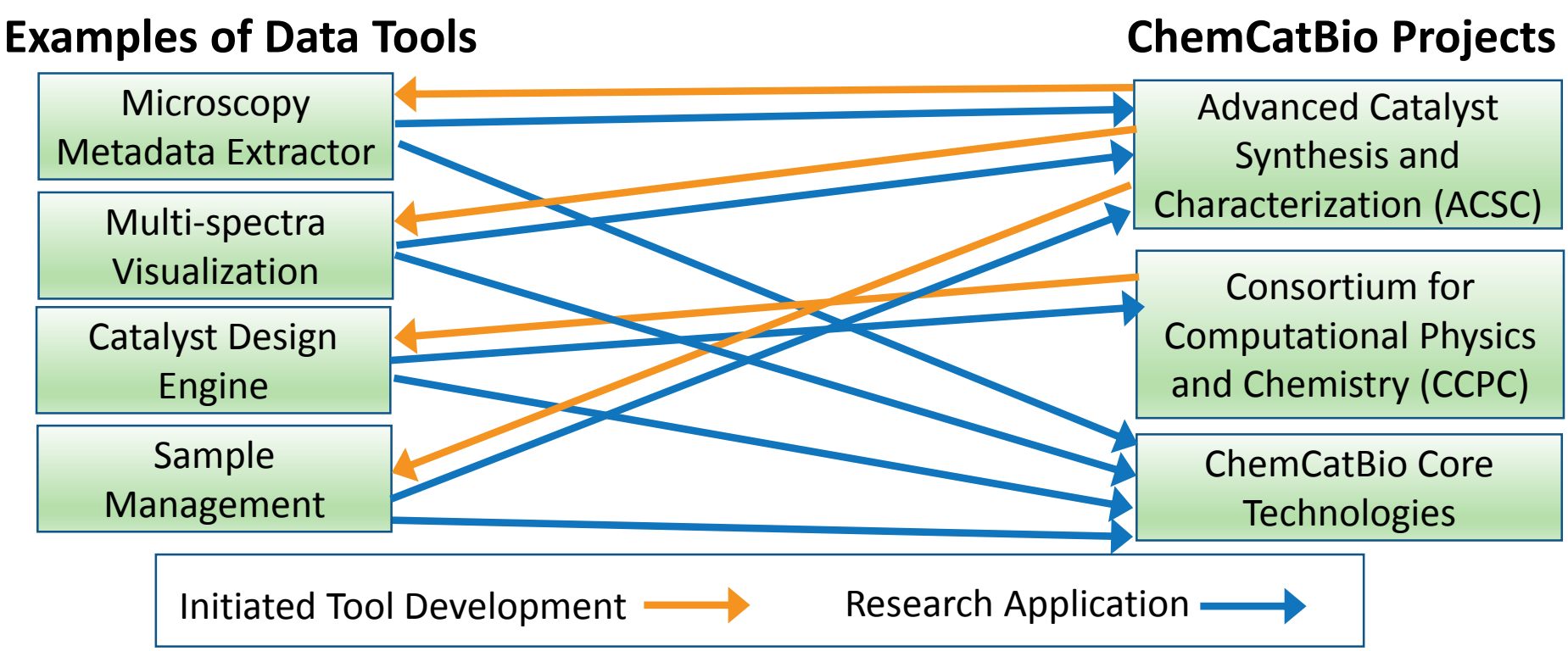


Management Approach

*Develop tools responsive to researcher needs through **researcher-centric approach***

Task 1: Build DataHub Infrastructure and Tools
- Build DataHub framework
- Develop plug-ins for storing, searching, and processing
- Develop advanced analytics tools

Task 2: Interface with Researchers
- Solicit regular researcher feedback to guide tool development
- Ensure deliverables are responsive to researcher needs

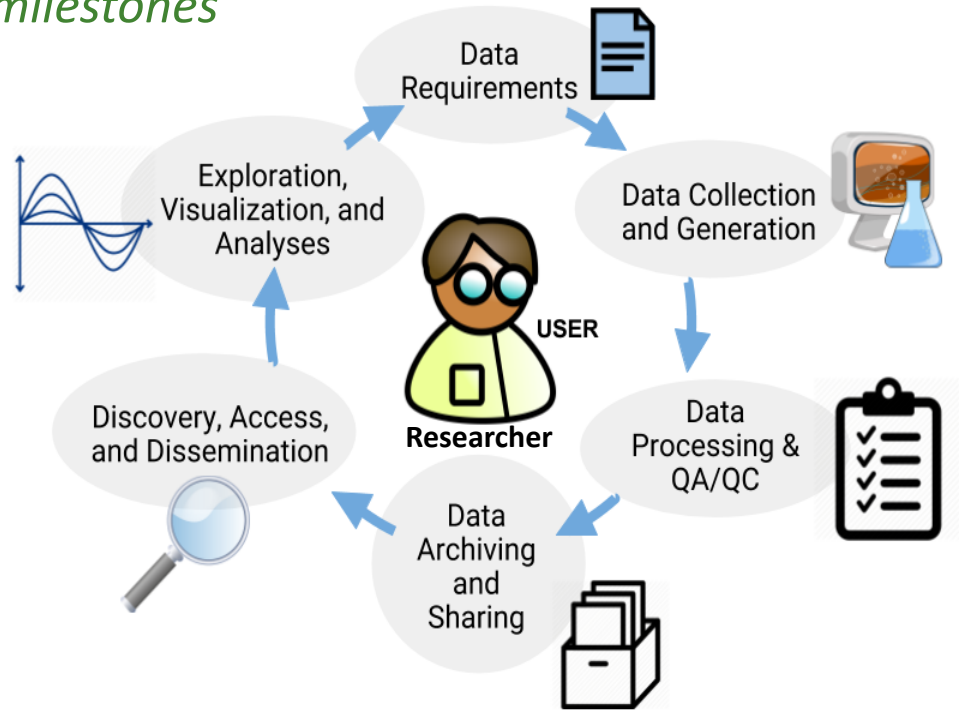


Management Approach

*Develop tools responsive to researcher needs through **researcher-centric approach***

FY18 Go/No-Go: The need for additional scope in FY19 will be assessed based on feedback from the ChemCatBio technical teams and steering committee.

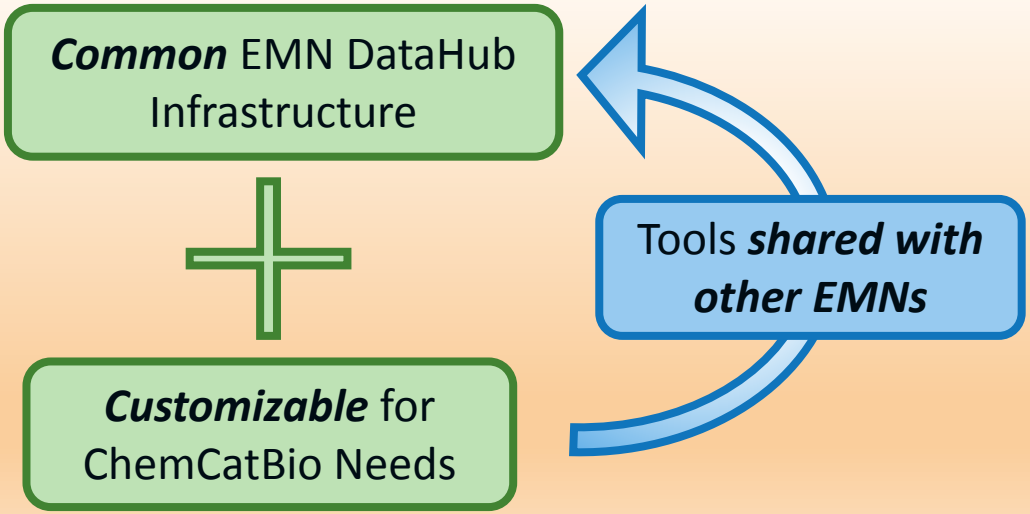
- *Led Data needs discussion at face-to-face meeting and teleconference and solicited specific researcher input through survey*
- *Feedback clearly indicated that **greatest value** is in **tool development***
- *Applied results to define FY19/20 milestones*



Technical Approach: Critical Challenges and Risk Mitigation

Critical Challenges

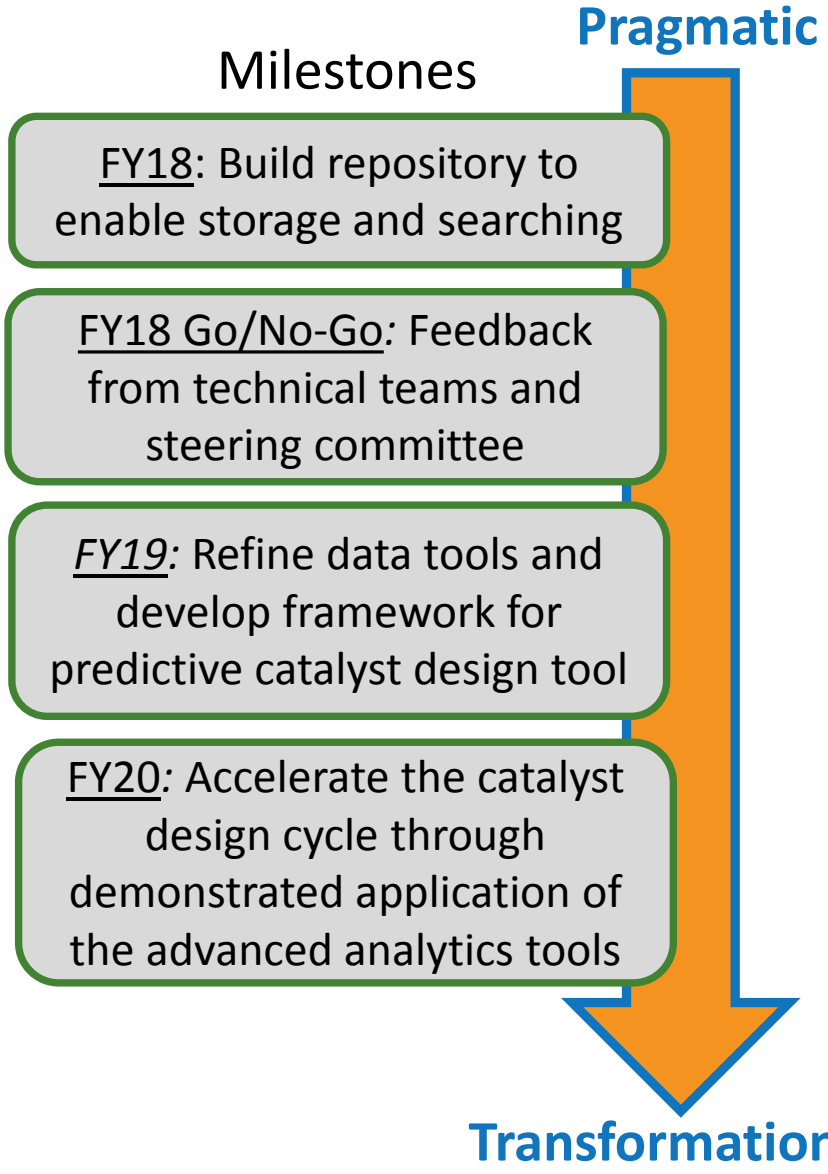
- Sharing Data
- Reducing Redundancy
- Accelerating Catalyst Design



Risk Mitigation

- Utilized by researchers
  - ➢ Integrate functionalities responsive to researcher needs
- Eliminates extra burdens
  - ➢ Develop plug-ins that upload large amounts of data with minimal researcher input

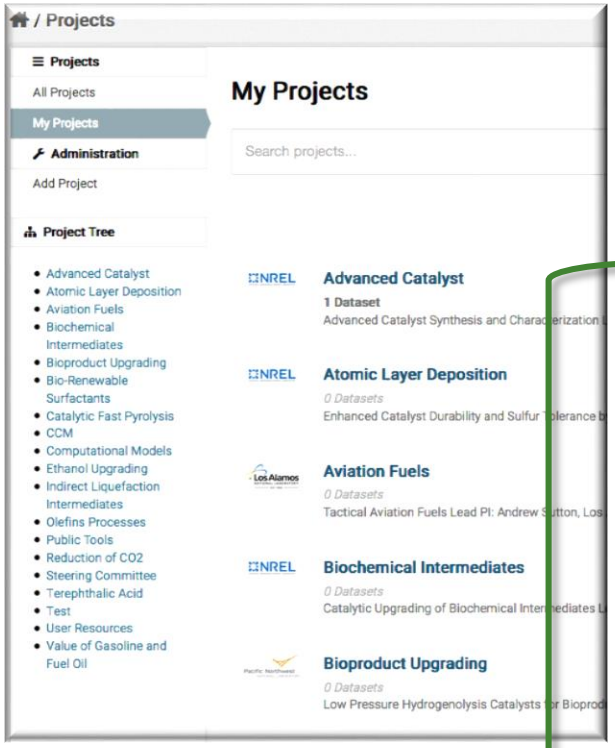
Technical Approach: Milestones and Success Indicators

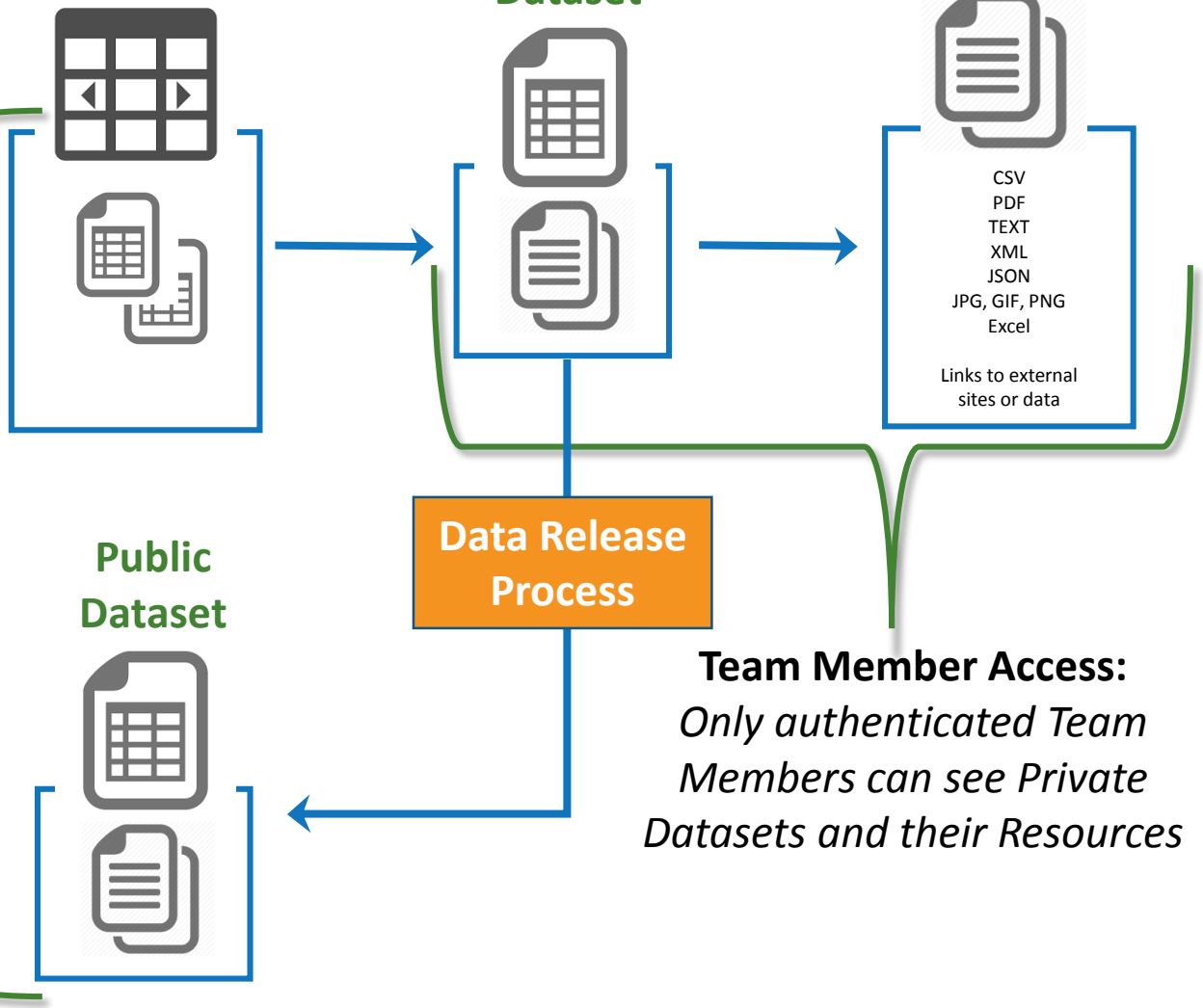


Critical Success Factors:

1. Data generated by researchers and industry partners can be **securely stored**, **easily searched**, and **quickly shared** with team members
2. Data is **processible** into formats that provide **key actionable information**
3. Data repository facilitates **dissemination** of ChemCatBio research through **controlled, public access**
4. Provide **predictive** capabilities that **accelerate** the **design of high-performing catalysts**

Progress: Centralized and Secure Data Repository



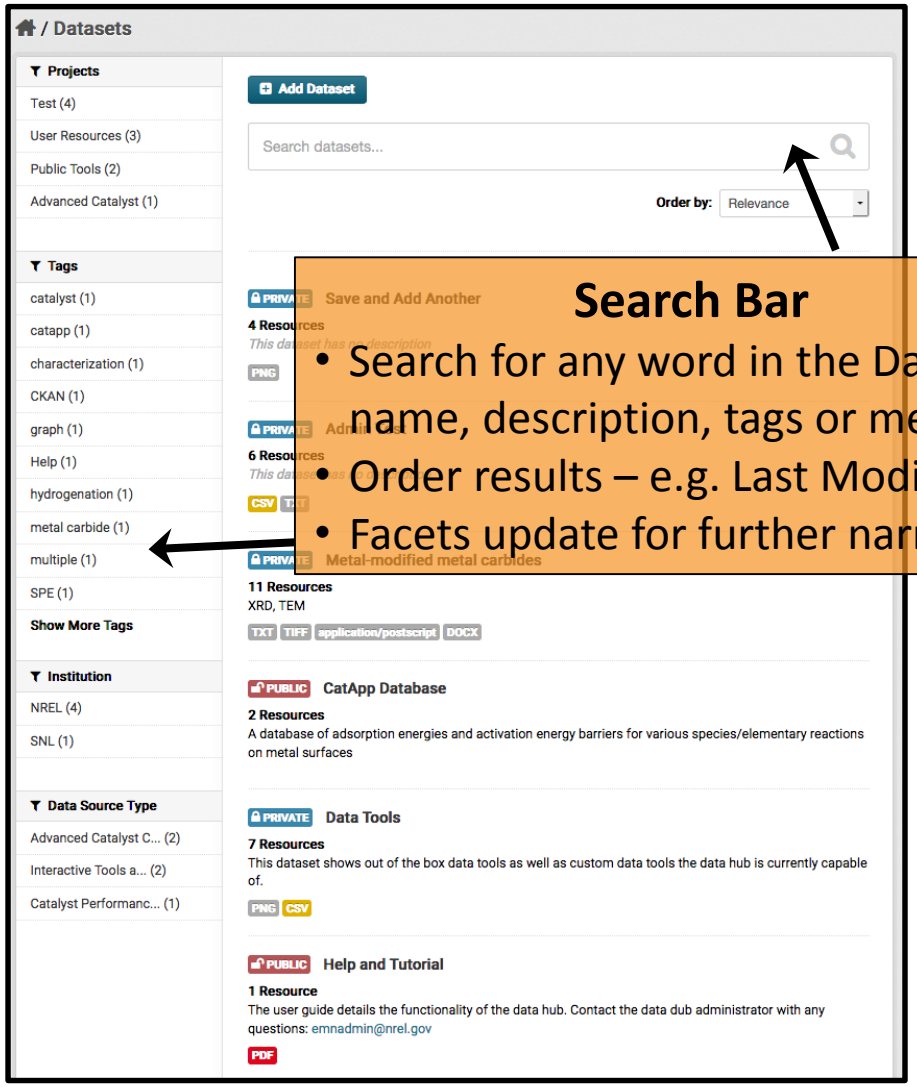


Public Access:
The public can see Project names, descriptions and abstracts. Public Datasets are also accessible.

Team Member Access:
Only authenticated Team Members can see Private Datasets and their Resources

Progress: Efficient User Data Search

Users can search across all accessible data

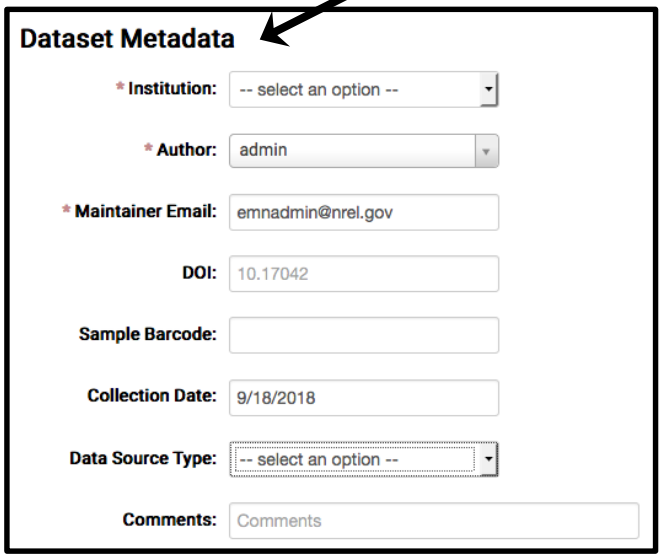


Search Bar

- Search for any word in the Dataset name, description, tags or metadata
- Order results – e.g. Last Modified
- Facets update for further narrowing

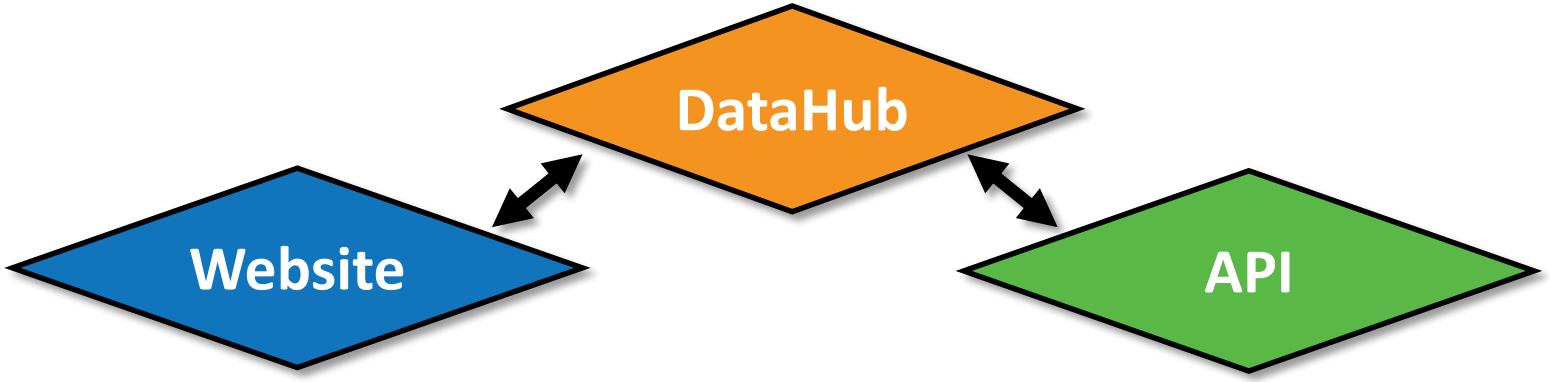
Metadata

- Entered/extracted at data upload
- Selected based on researcher input



Progress: Easy Access and Utilization of Data

Data Access and Application:

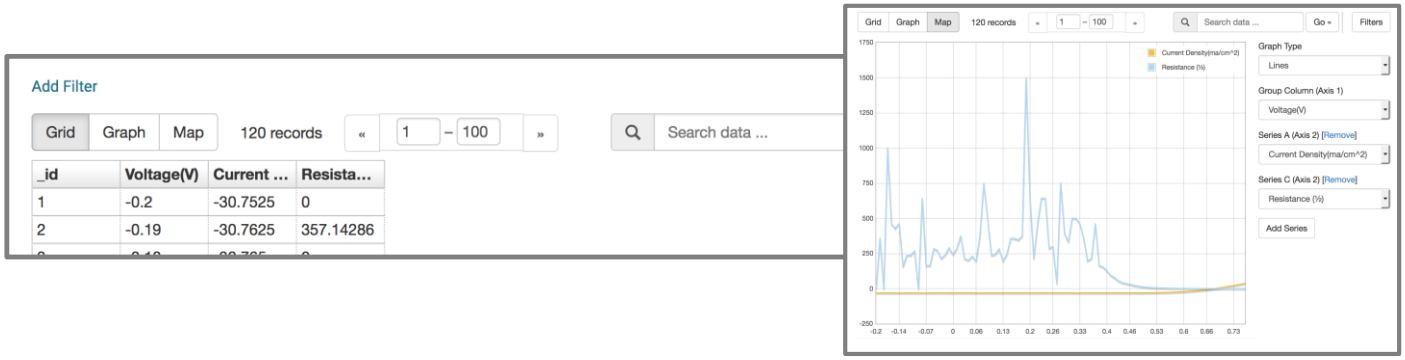


Provides user-friendly access for data and data tools

Enables building separate apps (e.g., Python notebooks) for visualization and analysis

Universal EMN Data Tool: Quick visualization, filtering, and searching

- Grid format or dynamic plotting of structured data (e.g., CSV files)

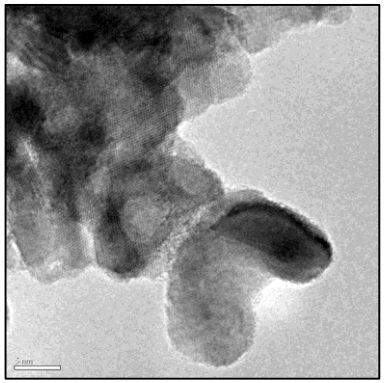


Progress: Fast Data Upload

Custom data tools address the **unique data needs** of ChemCatBio researchers

Automated Microscopy Metadata Extraction

- **Requested** by **ACSC** project team
- Enables **fast, batch data upload** and automatic extraction of instrument-specific metadata
- Enables **cross-institution collaboration** through advanced searching for image identification
- **Shared** across **all EMNs** through the EMN-Data Github repository



Original Image

Metadata Extraction Tool

Sample Name	**Ni_2P nanoparticle**
Acquisition Date	03/08/2017
Operator	Carrie Farberow
Microscope	FEI TEM
Magnification	2950000
…	

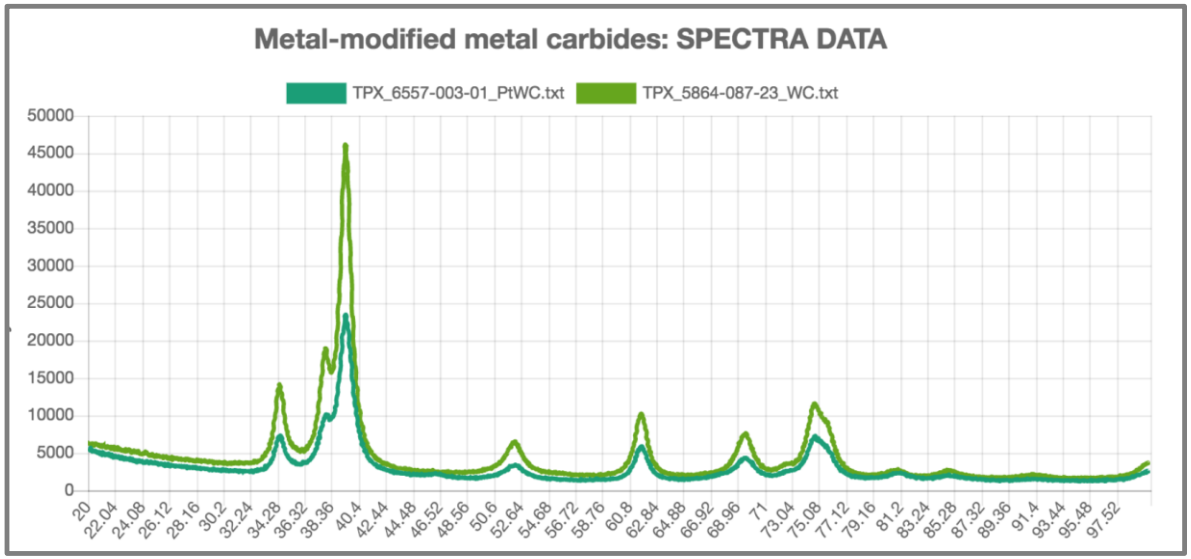
Extracted Metadata

Progress: Fast Data Visualization

Custom data tools address the **unique data needs** of ChemCatBio researchers

Multi-spectra Visualization

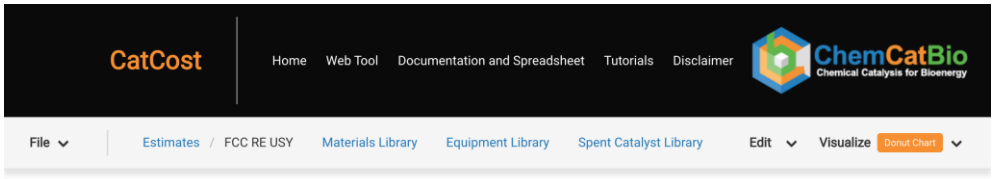
- **Requested** by **ACSC** project team
- Enables **rapid comparison** of data generated across institutions through **quick visualization** of **multiple spectral** data files in a **single plot**
- **Shared** across **all EMNs** through the EMN-Data Github repository

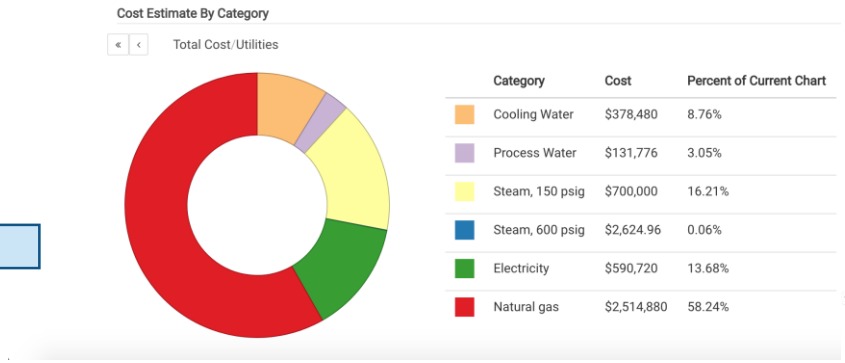


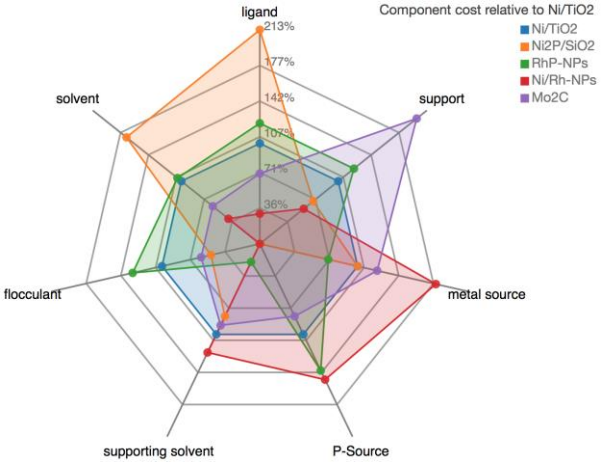
Progress: Facilitate Application of CatCost Tool

Integrated CatCost tool in DataHub for easy application in ChemCatBio research

- *Import materials libraries and estimates from the DataHub*

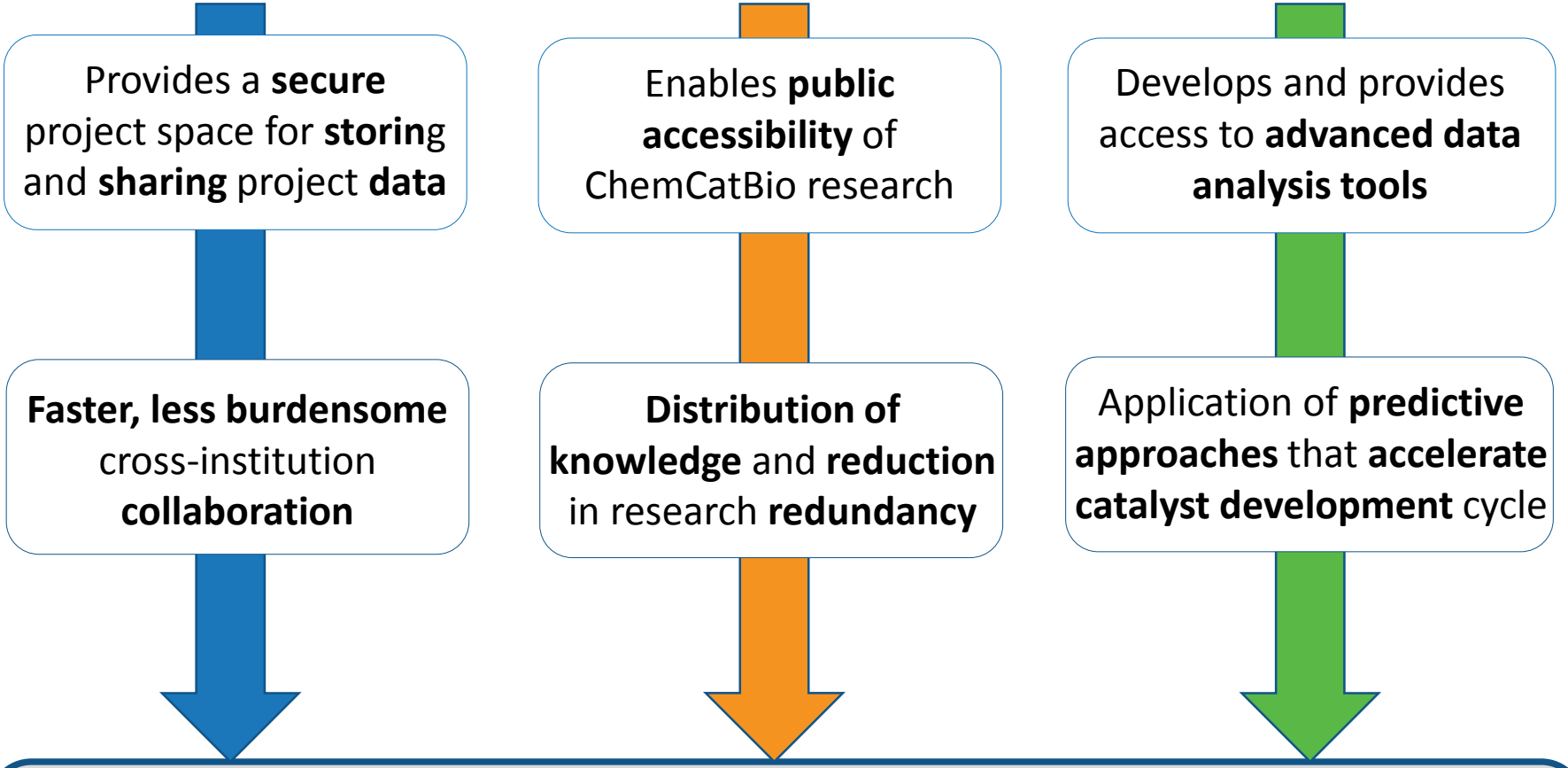






- *Export model outputs to the DataHub for archive and sharing*

Relevance: Faster, Less Costly Catalyst Development



BETO 2019 MYP **"Critical Barrier"**: **Reduce** the **time and cost** to develop active, selective, low-cost and durable **real-world catalysts** to produce **desired end-products from biomass and waste resources**.

Relevance: Broadly Applicable Catalyst R&D Tools

This project develops and provides access to broadly applicable and transformative catalyst R&D tools

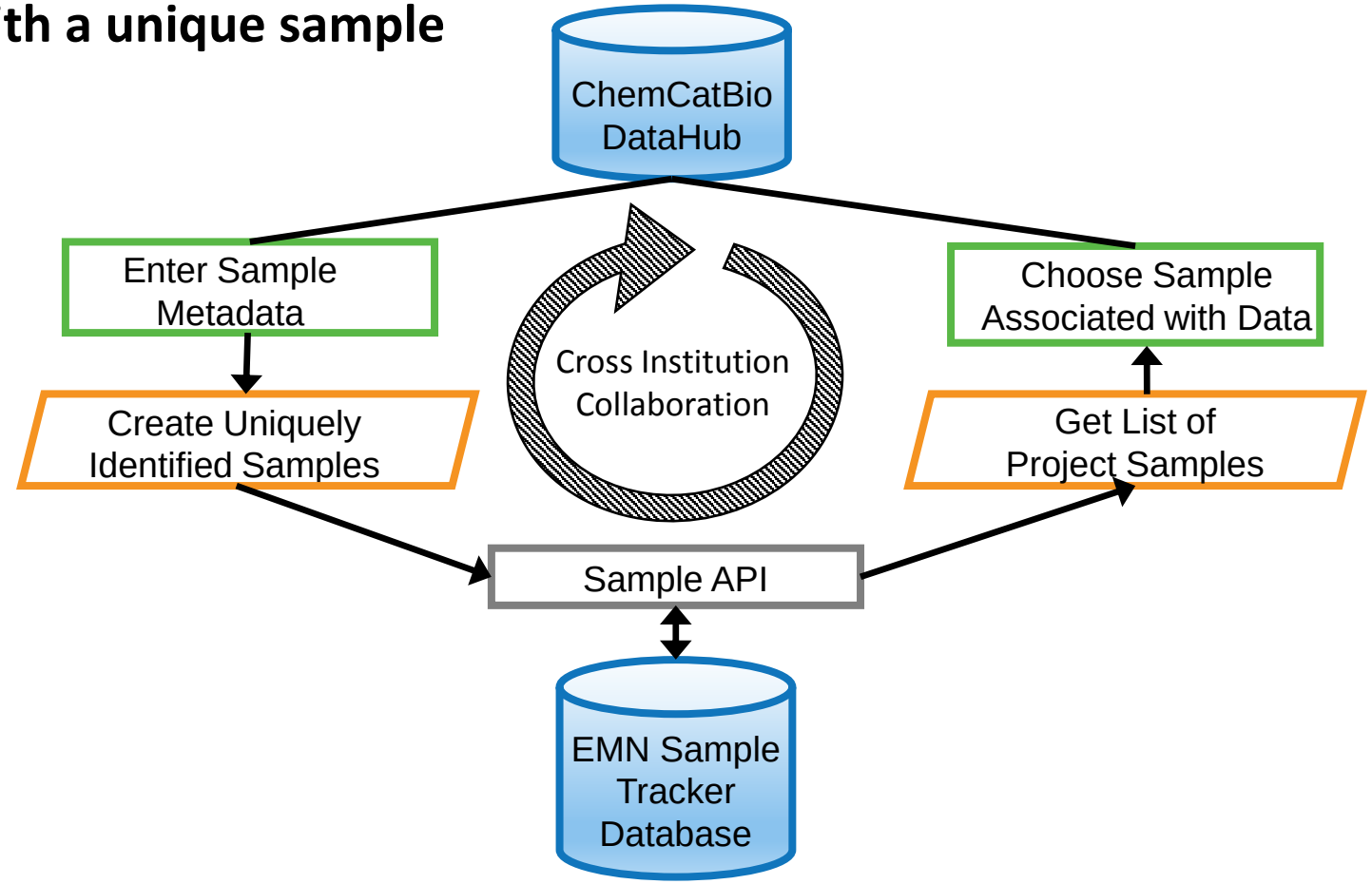
- Tools developed are **pathway-independent** and therefore **widely applicable** by industry for catalyst development
- **Public access** to both general and reaction-specific catalyst property data and associated analysis tools
- Centralized data storage and sharing location for ChemCatBio **DFA projects** creates immediate **value to industry partners**

Future Work: Sample Management

<u>Goal:</u> Researchers across institutions can share datasets and easily associate them with a unique sample

<u>Outcomes:</u>

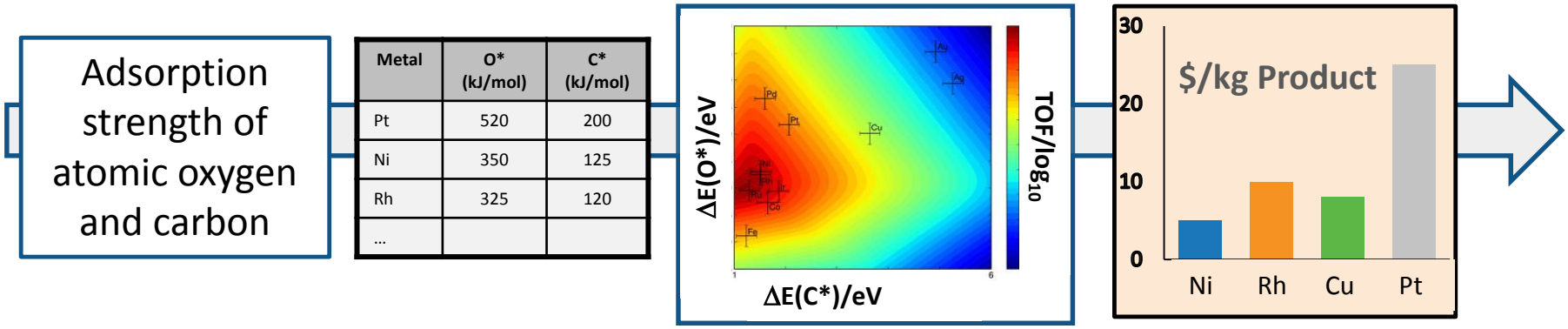
- ✓ **Reduces redundancy**
- ✓ **Increases knowledge gained**



Future Work: Catalyst Design Engine

Conventional State-of-the-Art Computational Catalyst Screening Process

Example: Methane Steam Reforming



Process Deficiencies

- Redundancy in descriptor value calculations
- Candidate materials often limited to expensive noble metals
- Difficult to consider economics for pre-commercial materials
- Lack of known descriptors for many complex reaction chemistries

Future Work: Catalyst Design Engine

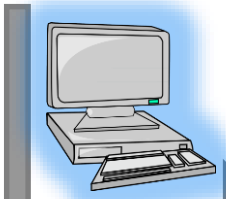
Integrated, broadly applicable, catalyst design tool that considers trade-off between performance and material cost to accelerate the design of high-performing, low-cost catalysts

Established Property-Performance Relationships

Computational Property Database

- Centralized, searchable compilation of published data
- Identification and fill-in of data gaps through CCPC collaboration
- Include integrated analysis and visualization tools

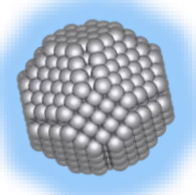
Leverage database and experimental collaborations for descriptor discovery



Predicted Performance of Diverse Materials

CatCost

- Predicted cost for pre-commercial materials
- Completed integration in DataHub in FY18



Optimized Low-cost, High-performing Catalysts for Targeted Synthesis and Testing

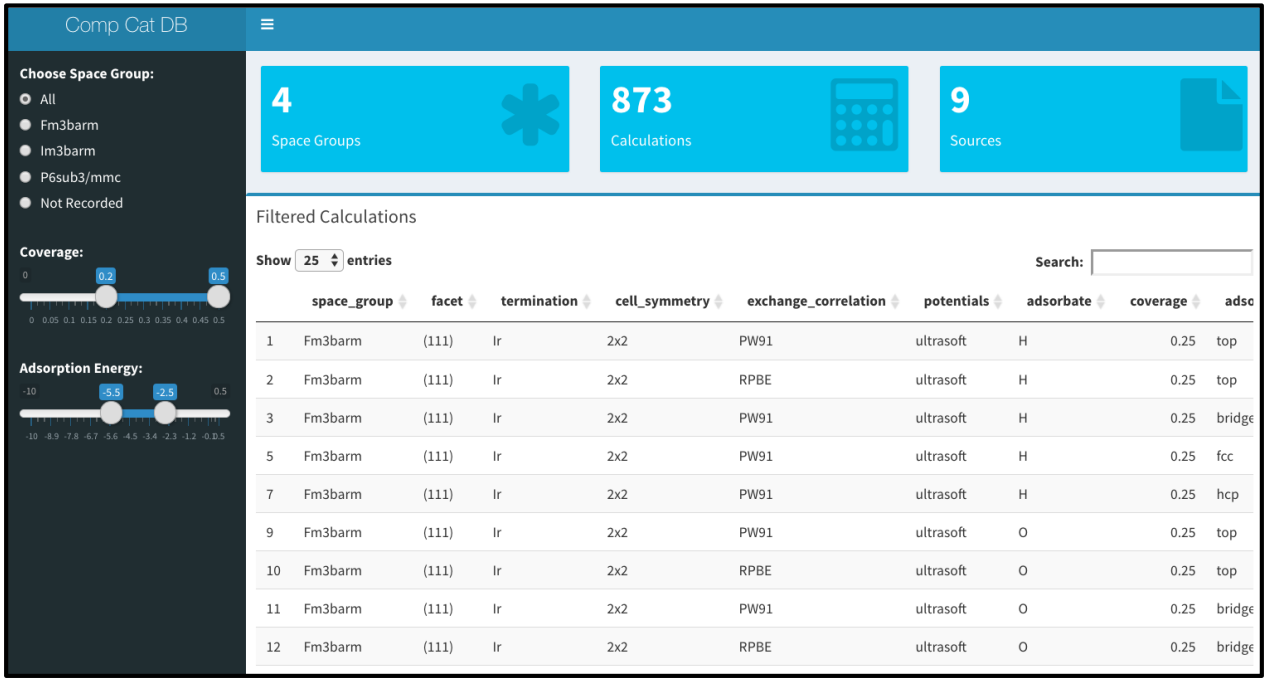
Future Work: Computational Catalyst Property Database

Progress to Date:

- Determined rules for data inclusion that maximize database utility while minimizing database compilation time
- Designed user interface framework
- Created prototype filter and search functions
- Populated database with initial set of 900+ calculations from literature

Next Steps:

- Expand data an order of magnitude (FY19Q2-Q4)
- Refine user interface (FY19Q2-Q3)
- Add analysis features, including visualization and plotting (FY20)



Summary

Project Goal: **Reduce** the **time and cost** for **ChemCatBio** and the **bioenergy industry** to develop **real-world catalysts** for the production of **desired end-products from biomass and waste resources** by providing:

1. Secure **data storage, sharing, and analysis** for cross-institution collaboration and **knowledge dissemination**
2. Development and application of **advanced analytics tools** that provide **predictive catalyst development** capabilities

Approach: **Researcher-centric** to ensure that the tools developed are **responsive** to researcher needs and **collaborative** with other **EMN data teams** to **eliminate redundancy**

Future work defined **based on researcher feedback** focuses on development of transformational tools including a **pathway-independent integrated catalyst design engine** that considers critical **trade-off** between **predicted performance** and catalyst **material cost** to **accelerate the design of optimized catalyst** formulations for a diversity of targeted end-products.

Acknowledgements

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ChemCatBio Researchers

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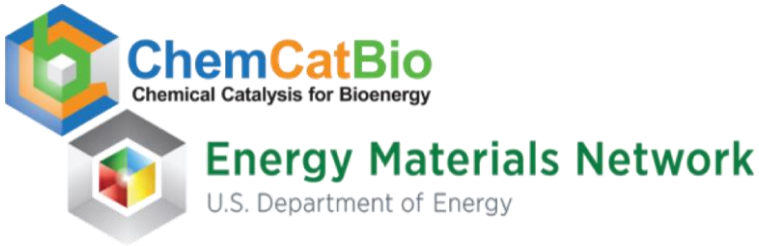
This work was performed in collaboration with the Chemical Catalysis for Bioenergy Consortium (ChemCatBio, CCB), a member of the Energy Materials Network (EMN)



Thank you.

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