

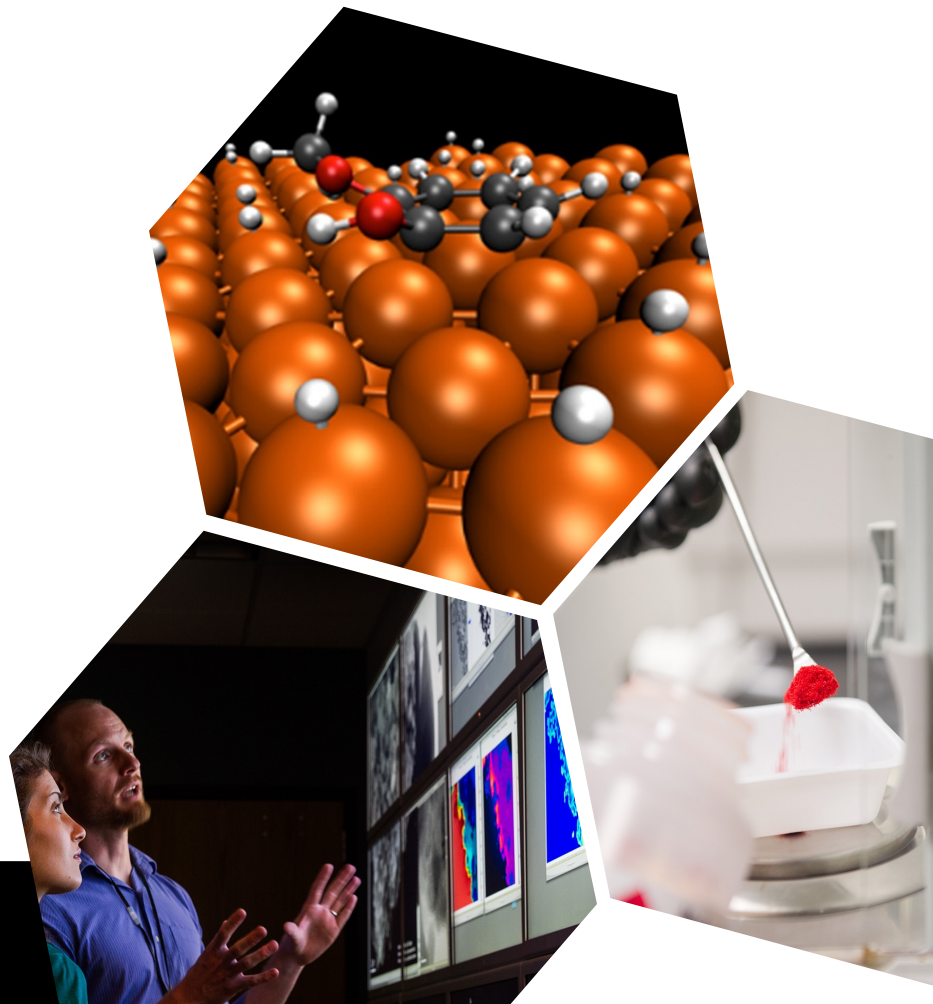


Reduce, Reuse, Recycle: Data Benchmarking and Accessibility for Faster Research With the Catalyst Property Database

October 13, 2021

ChemCatBio Webinar Series

Kurt Van Allsburg, NREL



Housekeeping

- Attendees will be in listen-only mode
- Audio connection options:
 - Computer audio
 - Dial in through your phone (best connection)
- Use the Q&A panel to ask questions
- Technical difficulties? Contact Erik Ringle through the chat section, lower right of your screen
- Recording will be available at: <https://www.chemcatbio.org/webinars.html>

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Today's Speaker



Kurt Van Allsburg

Catalyst Scientist, National
Renewable Energy Laboratory

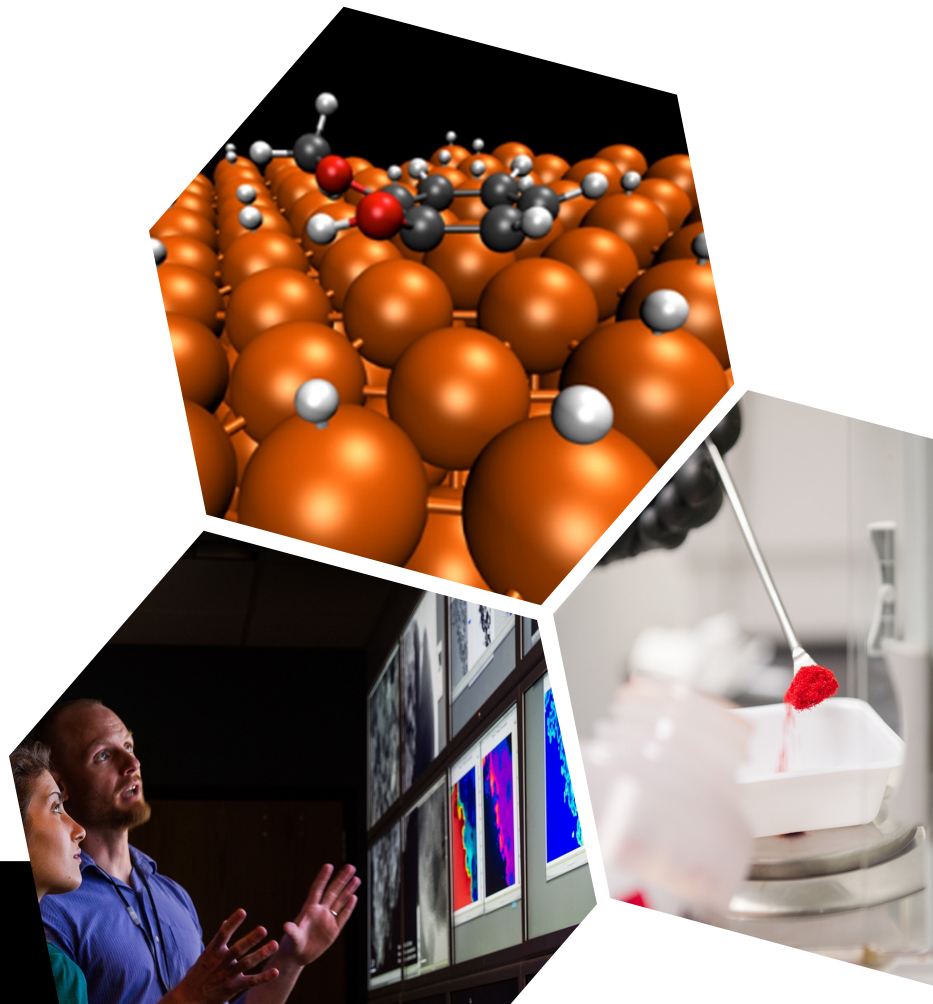


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The Chemical Catalysis for Bioenergy consortium (ChemCatBio)

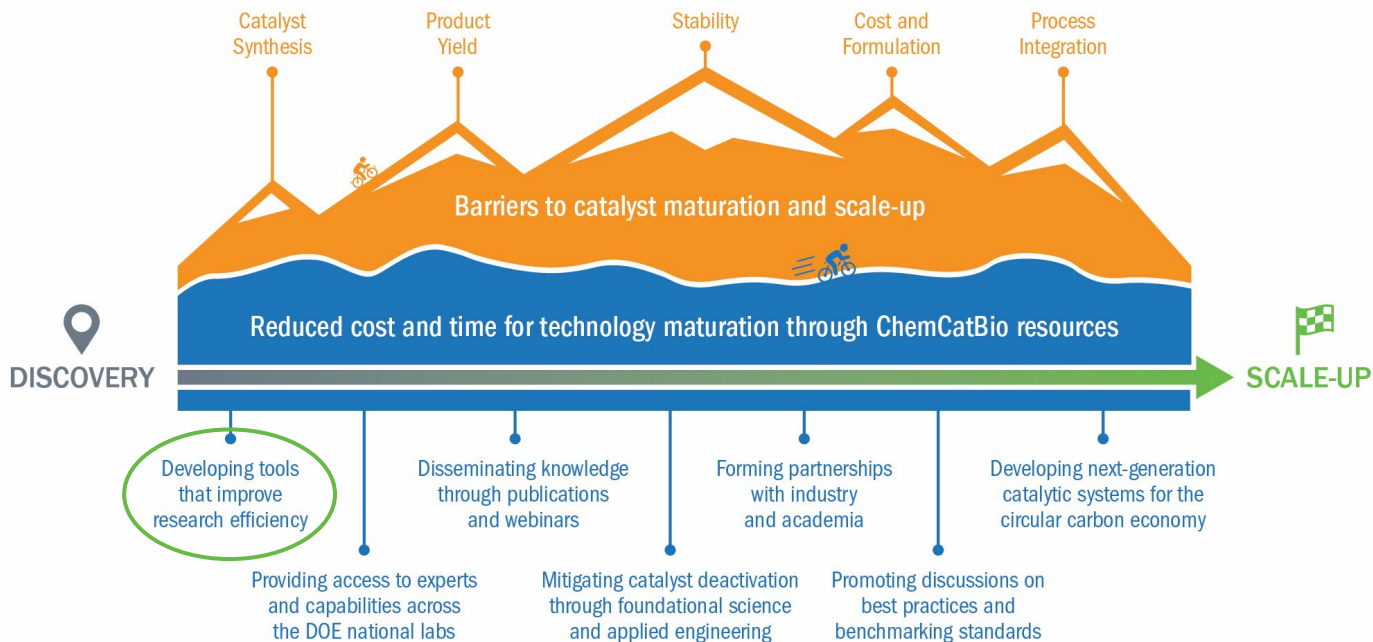
Accelerating the catalyst and process development cycle

<https://chemcatbio.org>

Subscribe to our newsletter **The Accelerator**

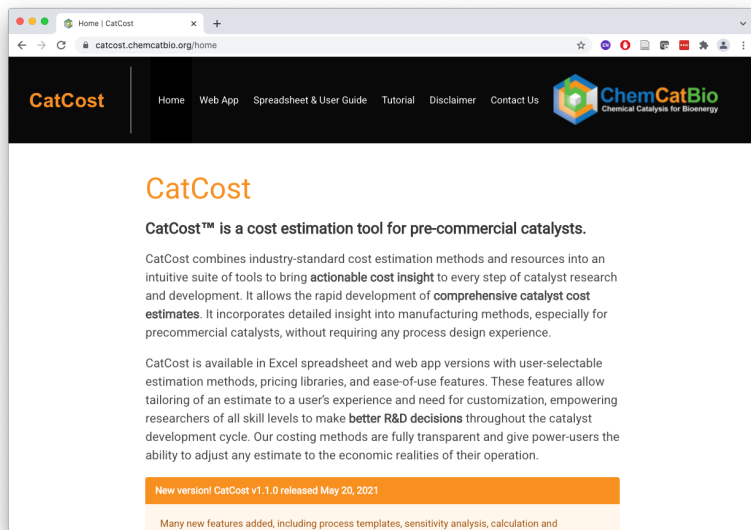
ChemCatBio: Accelerating Catalyst Discovery

The path to catalyst deployment is slow and difficult.



ChemCatBio is accelerating the catalyst and process development cycle.

Released in 2018: CatCost



CatCost™

a free catalyst cost estimator

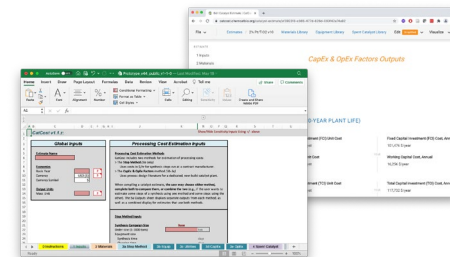
released in 2018

major update in May 2021

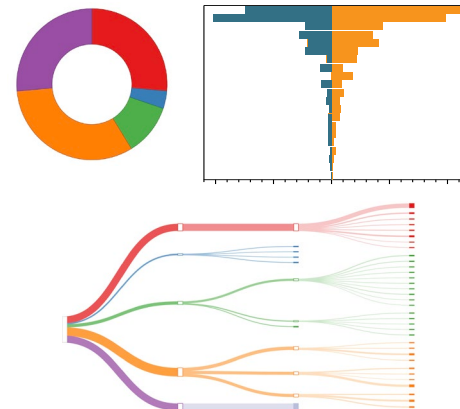
+ new mailing list

catcost.chemcatbio.org

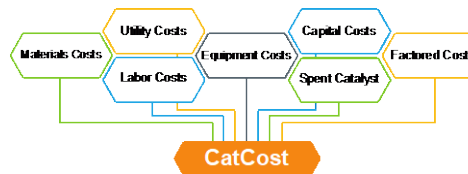
Excel and web app versions, with Python interconversion



Advanced visualizations built in



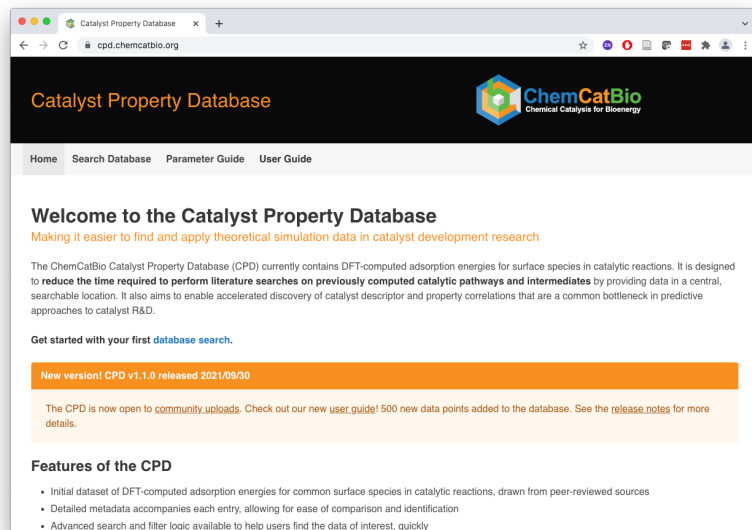
Detailed capital and operating costs



PI: Fred Baddour

Team Members: Kurt Van Allsburg, John Super, Eric Tan, Lesley Snowden-Swan, John Frye, James White, Joshua Schaidle, Michael Talmadge, Jesse Hensley, Susan Habas, Nicholas Wunder, Kenny Gruchalla, John Yarbrough, Kristi Potter, Matt Jankousky, Andy Young

Today's Webinar: the Catalyst Property Database



The Catalyst Property Database

a free database for catalyst research

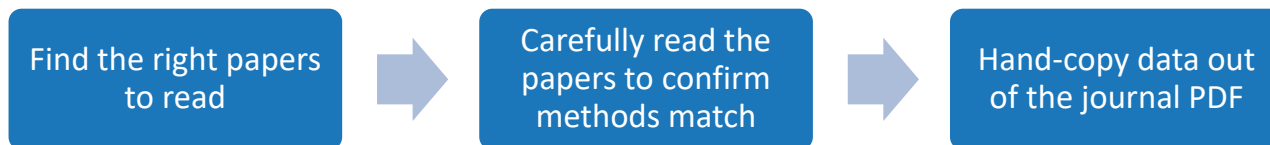
released in 2020

opened to external contributions Sept 2021

cpd.chemcatbio.org

Why build a catalyst database?

Problem: Finding the right catalysis data in the literature is often slow and cumbersome



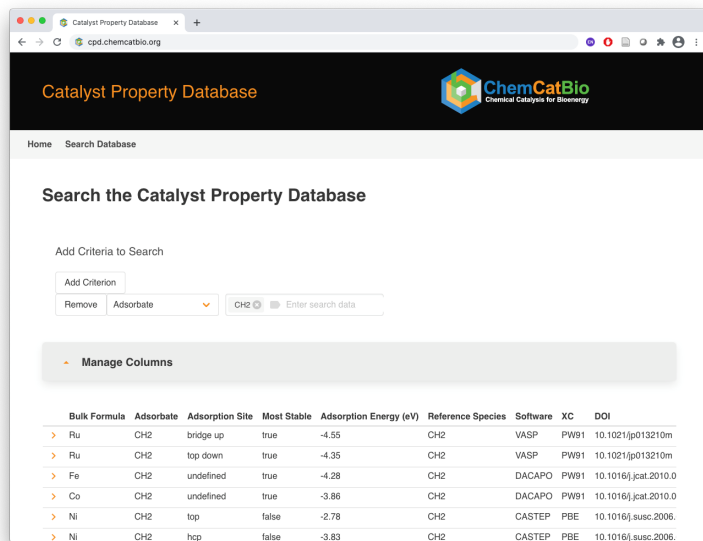
Result: Because of the challenges in finding **reliable, directly comparable** datasets, it's often easier to just **collect/compute it yourself (duplication of effort, \$\$\$, time)**



Our goal: Reduce, Reuse, Recycle

Accelerate catalysis research by making it easier to find and reuse catalyst data

Our answer: make catalyst data more accessible



The screenshot shows the Catalyst Property Database website. The header includes the logo and name "ChemCatBio Chemical Catalysis for Bioenergy". Below the header is a search bar with the text "Search the Catalyst Property Database". There are options to "Add Criteria to Search" and "Manage Columns". A table of catalyst data is displayed below the search interface.

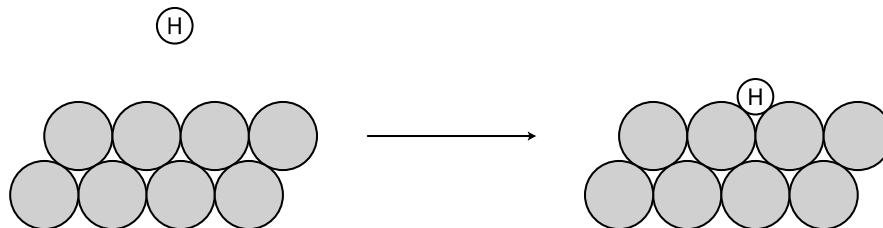
Bulk Formula	Adsorbate	Adsorption Site	Most Stable	Adsorption Energy (eV)	Reference Species	Software	XC	DOI
> Ru	CH2	bridge up	true	-4.55	CH2	VASP	PW91	10.1021/pj013210m
> Ru	CH2	top down	true	-4.35	CH2	VASP	PW91	10.1021/pj013210m
> Fe	CH2	undefined	true	-4.28	CH2	DACAPO	PW91	10.1016/j.jcat.2010.0
> Co	CH2	undefined	true	-3.86	CH2	DACAPO	PW91	10.1016/j.jcat.2010.0
> Ni	CH2	top	false	-2.78	CH2	CASTEP	PBE	10.1016/j.susc.2006.
> Ni	CH2	hcp	false	-3.83	CH2	CASTEP	PBE	10.1016/j.susc.2006.

Data in the CPD is:

- Centralized
 - Enabling faster comparisons
- Searchable
 - Search dozens of metadata fields directly
 - Find the right data faster
- Publicly accessible to view and upload
 - Uploads subject to quality control

- Data types:**
- Computational catalysis (initial focus)
 - Catalyst characterization
 - Reaction performance

What sort of catalyst property data?



At initial release: Density functional theory-computed adsorption energies for intermediates on catalyst surfaces, from peer reviewed journals

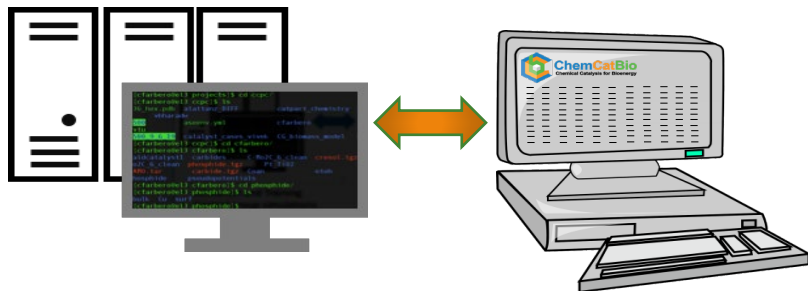
Long-term goals:

- Add new data types to enable scaling relation and reactivity descriptor discovery
- Experimental and computational results
- Catalyst property and preparation details
- Researcher-users of the CPD to guide data types and structure

Applications of the CPD

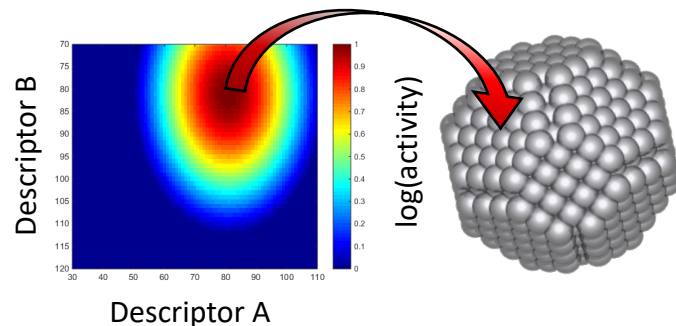
Benchmarking & Validation

Researchers wanting to check their results

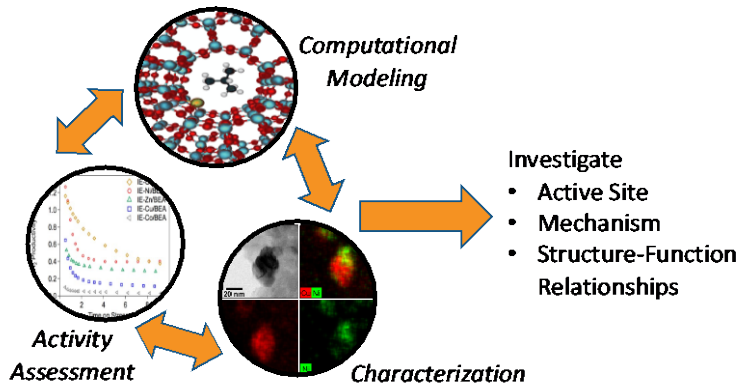


Catalyst Screening

Applying reactivity data to identify new target compositions

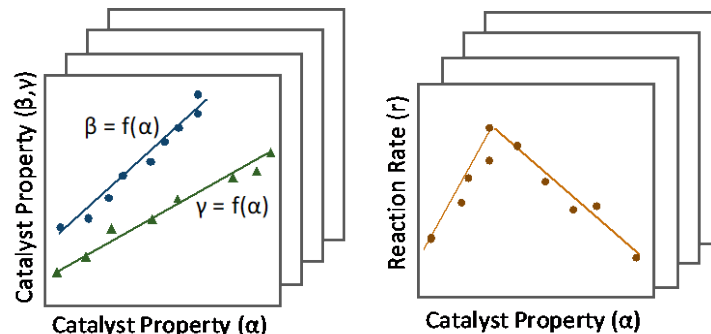


Interpretation of Experimental Trends



Discovery of Scaling Relations and Reactivity Descriptors

Harnessing the power of a large, central database



✓ **Part I: Why we built it**

Part II: How we built it (and why you should care)

... and examples, upcoming additions, etc.

The CPD Team

CHEM TEAM



Kurt Van Allsburg

PI
Experimentalist



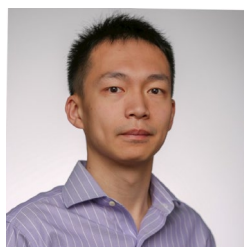
Carrie Farberow

Co-investigator
Computational
researcher



Sean Tacey

Computational
researcher



Qiyuan Wu

Experimentalist
Experienced web
developer

DEV TEAM



Nalinrat Guba

Software engineer
(previously at Oracle)



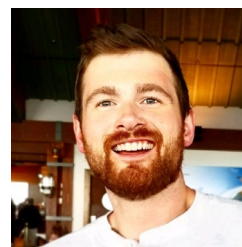
Alicia Key

Software engineer with
computational
chemistry experience



Rachel Hurst

Technical project lead,
system architect



Tom King

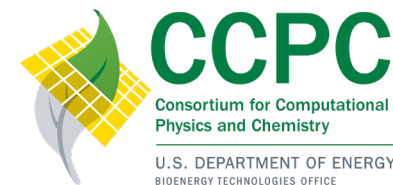
UI/UX designer

Advisors:

Josh Schaidle, CCB Director

Nick Wunder, NREL

Collaborations:



CatCost

The CPD: Fast, simple searching

Catalyst Property Database

Home Search Database

Search the Catalyst Property Database

Add Criteria to Search

Add Criterion

Remove Adsorbate CH2 Enter search data

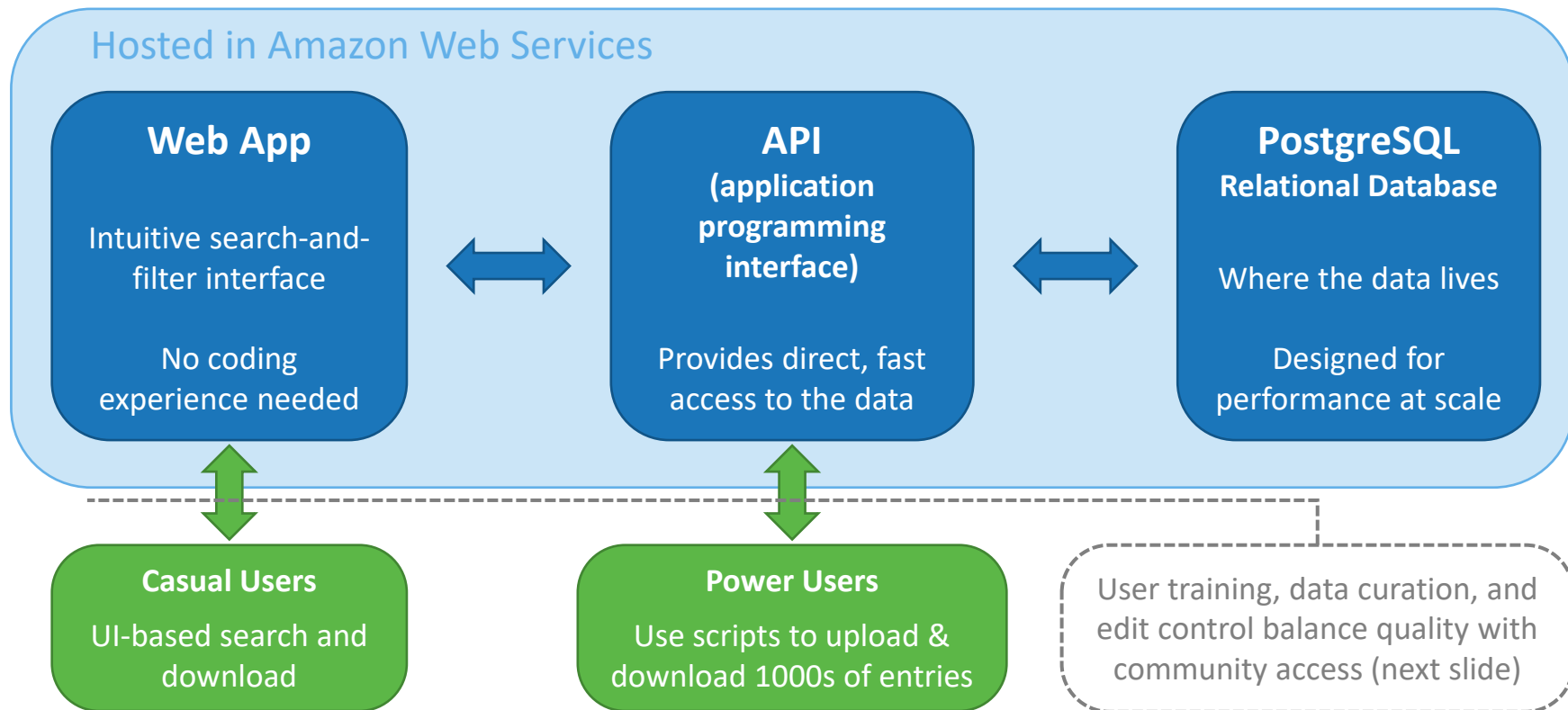
Manage Columns

	Bulk Formula	Adsorbate	Adsorption Site	Most Stable	Adsorption Energy (eV)	Reference Species	Software	XC	DOI
>	Ru	CH2	bridge up	true	-4.55	CH2	VASP	PW91	10.1021/jp013210m
>	Ru	CH2	top down	true	-4.35	CH2	VASP	PW91	10.1021/jp013210m
>	Fe	CH2	undefined	true	-4.28	CH2	DACAPO	PW91	10.1016/j.jcat.2010.0
>	Co	CH2	undefined	true	-3.86	CH2	DACAPO	PW91	10.1016/j.jcat.2010.0
>	Ni	CH2	top	false	-2.78	CH2	CASTEP	PBE	10.1016/j.susc.2006.
>	Ni	CH2	hcp	false	-3.83	CH2	CASTEP	PBE	10.1016/j.susc.2006.

- Search updates live as you add criteria
- Designed for use by both computational and experimental researchers
- Simple interface

CPD Architecture: Designed for Scale

The CPD uses a modern design for fast performance as the database grows



Structuring the data

Developed a data structure for computed adsorption energies

Field	Data Type	Required Field?
<u>Material Properties</u>		
Formula	String	Yes
Primary Class	String	No
Secondary Class	String	No
Stretched?	Boolean	Yes, default False
Compressed?	Boolean	Yes, default False
Space Group	String	No
Lattice Constants (3)	Numeric	No
<u>Surface/Particle Properties</u>		
Nanoparticle Size	Numeric	No
1st Layer Composition	String	No
2nd Layer Composition	String	No
Facet	String	No
Termination	String	No
Cell Symmetry	String	No
<u>Methods</u>		
Software	String	Yes
Exchange correlation	String	Yes
Potentials	String	No
Basis Set	String	Yes
SpinPol?	Boolean	No
ZPE?	Boolean	No
Fixed Substrate?	Boolean	No

Field	Data Type	Required Field?
<u>Adsorbate and Reference Species</u>		
Adsorbate	Table	Yes
Adsorption Site	String	No
Coverage	Numeric	No
Reference Species (multiple)	Table	At least one entry required
Reference Species coefficient	Numeric	Yes
<u>Metadata</u>		
DOI	String	Yes
Notes	String	No
User	String	Yes
<u>Adsorption Energy Data</u>		
Adsorption Energy	Numeric	Yes
Most Stable?	Boolean	Yes, default True

This is key to our goal of helping users find **the right data, faster**

We'll work with users to define structures for new data types

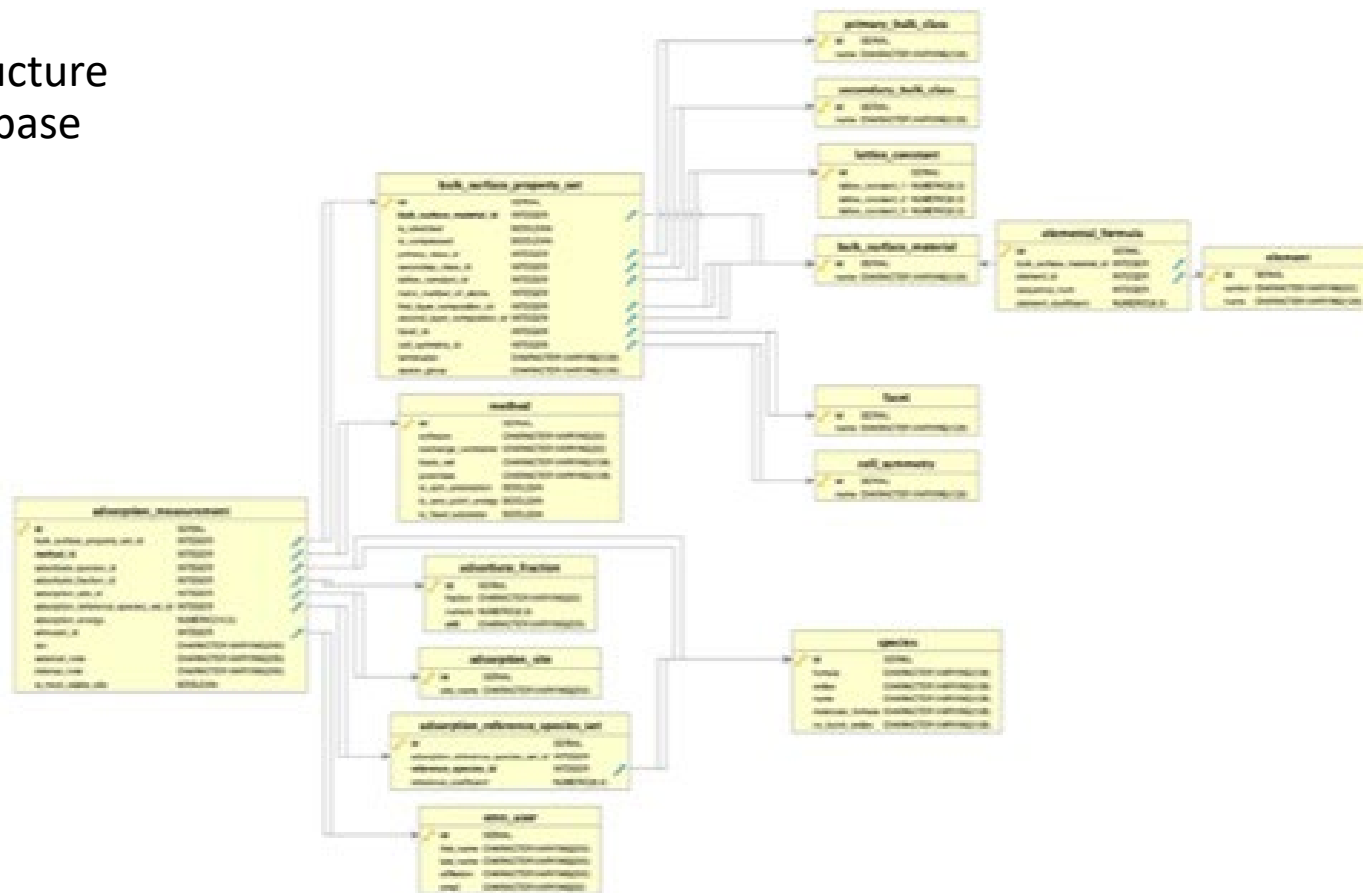
Structuring the data

Converted the data structure into a PostgreSQL database

Database ready to efficiently scale up to millions of entries

We can do this faster for new data types (characterization, synthesis, reactor performance)

1....2....n....



Parameter Guide for non-experts...

- Making computational chemistry results accessible to more people
- Explaining ourselves if we've been unclear (it happens)

The screenshot shows a web browser window with the URL `cpd.chemcatbio.org/parameter-guide`. The page title is "Catalyst Property Database" and the logo for "ChemCatBio Chemical Catalysis for Bioenergy" is in the top right. A navigation bar includes "Home", "Search Database", "Parameter Guide" (which is active), and "User Guide".

CPD Parameter Guide

This page gives an explanation for the parameters included in CPD entries. The CPD currently contains density functional theory-computed surface adsorption energies. The parameters reflect this application.

Bulk Properties

The properties of the bulk material from which a surface slab or cluster model has been generated for the adsorption energy calculation.

Bulk Formula

The chemical formula of the bulk material.

String Required

Primary Class

Metadata describing primary characteristics of the bulk material, such as "transition metal".

String

Stretched?

Some calculations introduce a bulk lattice deformation. This field indicates whether the lattice was stretched relative to its relaxed (optimized) lattice parameters.

Boolean Required

Secondary Class

Metadata describing secondary characteristics of the bulk material, such as "bulk alloy".

String

Lattice Constants, Å (x3)

Compressed?

Some calculations introduce a bulk lattice

...and a User Guide for all

- Explanation of features
- Documentation for power-users and uploaders

The screenshot shows a web browser window with two tabs: 'Catalyst Property Database' and 'Searching the Database'. The address bar shows the URL 'cpd-docs.chemcatbio.org/#/search-database'. On the left is a navigation sidebar with the following items: 'Catalyst Property Database User Guide', 'Home', 'About the CPD', 'Contributors and Funding', 'Disclaimer', 'Searching the Database' (highlighted), '- Search', '- Add Search Criteria', '- Live Updating', '- Add More Criteria', '- Remove Criteria', '- Clear the Search', '- Review Results', '- Adsorbate and Reference Details', '- Detail View', '- Manage Columns', 'Parameter Guide', 'Uploading Data', and 'Curation'. The main content area is titled 'Searching the Database' and contains a 'Search' section with instructions on how to start a search. Below that is an 'Add Search Criteria' section with an example of adding an Adsorbate criterion. An inset image shows a close-up of the search interface with a dropdown menu for 'Adsorbate' showing options 'HNO', 'HNOH', and 'HNO' (selected). A 'Manage Columns' button is visible at the bottom of the inset.

Catalyst Property Database User Guide

Home

About the CPD

- Contributors and Funding
- Disclaimer

Searching the Database

- Search
- Add Search Criteria
- Live Updating
- Add More Criteria
- Remove Criteria
- Clear the Search
- Review Results
- Adsorbate and Reference Details
- Detail View
- Manage Columns

Parameter Guide

Uploading Data

Curation

Searching the Database

Search

Start a database search from the CPD homepage by clicking "Search Database" or going to https://cpd.chemcatbio.org/search_database.

Add Search Criteria

Add criteria to your search by clicking the "Add Criterion" button. Select the criterion you want using the "Select a criterion" dropdown. See the [CPD Parameter Guide](#) or the [Parameter Guide](#) page on this site for an explanation of each parameter that can be added as a search criterion.

Example of adding an Adsorbate="HNOH" search criterion (GIF):

Home Search Database Parameter Guide

Search the Catalyst Property Database

Add Criteria to Search

Add Criterion

Remove Adsorbate

Manage Columns

For many criteria, such as Adsorbate, you can continue adding multiple entries from the dropdown list. The CPD will return results matching ANY of the entries within a single criterion.

Standardizing data & creating rules

Created dictionaries of recurring entries, such as adsorbate/reference species, and rules for naming, data input/curation, etc.

Molecular Formula	Name	SMILES
O2 (g)	oxygen (g)	{OO}
OO	dioxygen	OO
O2	oxygen	O=O
HH	hydrogen (g)	{HH}
H2	hydrogen	[H][H]
O	oxygen, atomic	[O]
N2	nitrogen	N#N
CH3COOH	acetic acid	CC(=O)O
HCO	formyl	[CH]=O
CH2	methylene	[CH2]
COOH	carboxyl	[C](=O)O

Outcomes from dictionaries & data rules:

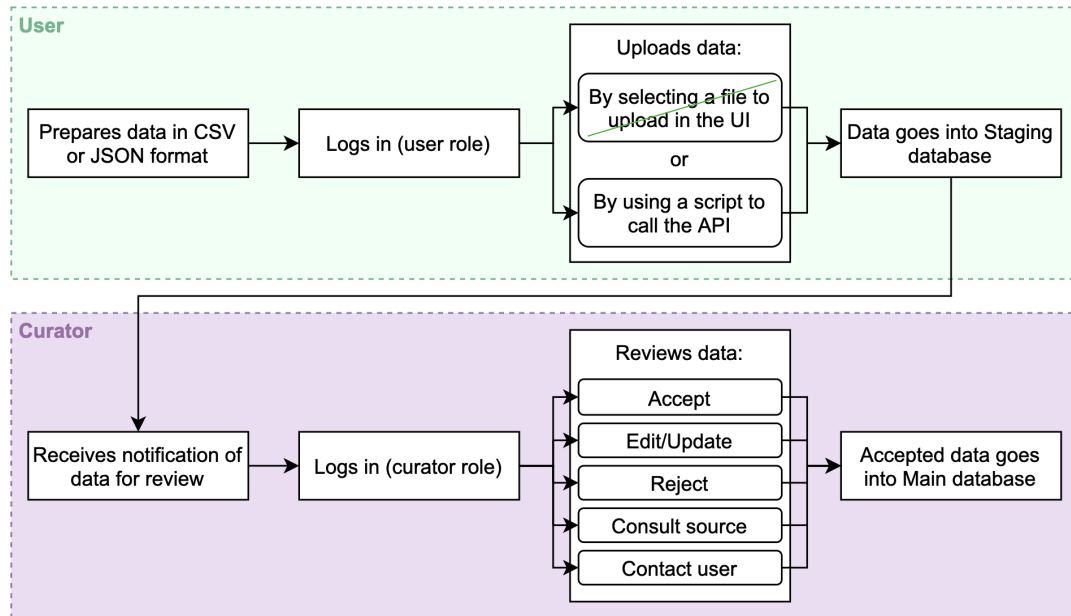
- Quality control
- Faster performance (fewer entries)
- Faster, easier search
- Gives users confidence in the data

Opening the CPD to community uploads

Sept 2021: CPD opened to uploads from the catalyst community

(previously, we added all data from the literature)

How data is uploaded and curated to ensure quality:



(still working out kinks here; it will get easier)

Hope to recruit a team of curators *a la* Wikipedia

Want to upload data? (adsorption energies)

Get started by cloning this repository.

github.com/NREL/cpd-batch-upload

Reach out anytime for help!

cpd@nrel.gov

The screenshot displays the GitHub repository page for `NREL/cpd-batch-upload`. The repository is public and has 111 commits. The file browser shows a commit by `kvanalls` with the following files:

File	Description	Last Commit
<code>cpdupload</code>	Update <code>__main__.py</code>	20 days ago
<code>docs</code>	Add documentation for authentication.	20 days ago
<code>input_examples</code>	Fix #N/A error in <code>CPD_data_example_from_API.json</code>	2 days ago
<code>integration_examples/VASP</code>	Add files via upload	21 days ago
<code>.gitignore</code>	Update <code>.gitignore</code>	20 days ago
<code>README.md</code>	Update <code>README.md</code>	20 days ago
<code>config.yaml</code>	Create <code>config.yaml</code> for production.	20 days ago
<code>mypy.ini</code>	MyPy and Black support	3 months ago
<code>pyproject.toml</code>	MyPy and Black support	3 months ago
<code>setup.py</code>	Update <code>setup.py</code>	21 days ago

The `README.md` file is selected, showing the following content:

cpdupload

Python 3 library for batch upload from files

Installation

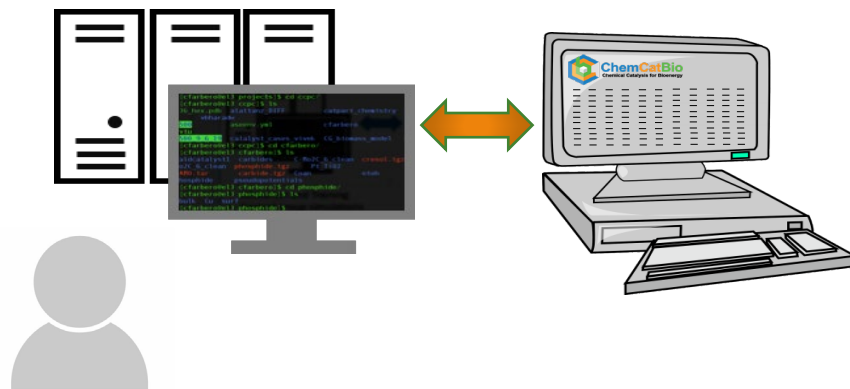
The right sidebar contains the following sections:

- About:** Part of the Catalyst Property Database. Python 3 library for batch upload from files. cpd.chemcatbio.org
- Releases:** 6 releases. Latest: Release 1.1.1 (7 days ago).
- Packages:** No packages published. [Publish your first package](#)
- Contributors:** 4 contributors: akey7, Alicia Key, ChemE-SeanT, kvanalls.

Two use case examples

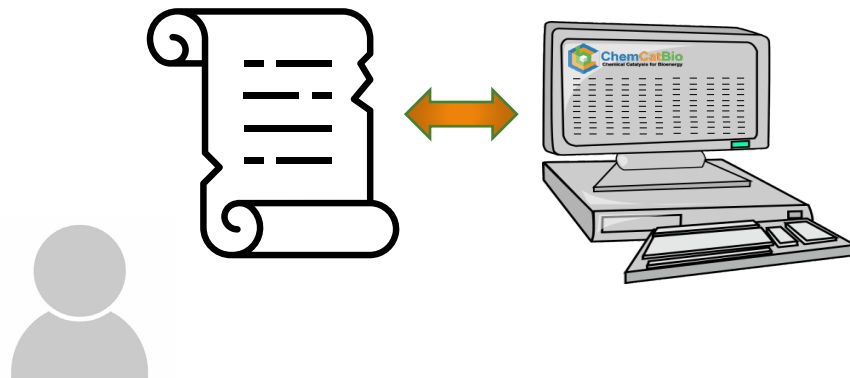
Use Case 1: Benchmarking

New computational chemistry graduate student: “leg up” on their project



Use Case 2: Benchmarking

Journal article reviewer: takes a lot of effort to do a “sanity check” on DFT papers



(we also hope editors and reviewers will encourage authors to upload their data)

Benchmarking is an important challenge facing the field

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ACS Catalysis

Perspective

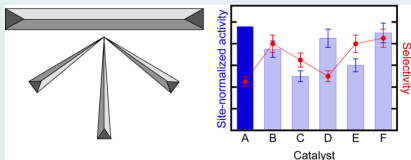
pubs.acs.org/acscatalysis

Toward Benchmarking in Catalysis Science: Best Practices, Challenges, and Opportunities

Thomas Bligaard,[†] R. Morris Bullock,^{*} Charles T. Campbell,[§] Jingguang G. Chen,^{*,||,⊥} Bruce C. Gates,[#] Raymond J. Gorte,[§] Christopher W. Jones,^h William D. Jones,ⁱ John R. Kitchin,^j and Susannah L. Scott^{*,k}

ABSTRACT: Benchmarking is a community-based and (preferably) community-driven activity involving consensus-based decisions on how to make reproducible, fair, and relevant assessments. In catalysis science, important catalyst performance metrics include activity, selectivity, and the deactivation profile, which enable comparisons between new and standard catalysts. Benchmarking also requires careful documentation, archiving, and sharing of methods and measurements, to ensure that the full value of research data can be realized. Beyond these goals, benchmarking presents unique opportunities to advance and accelerate understanding of complex reaction systems by combining and comparing experimental information from multiple, *in situ* and *operando* techniques with theoretical insights derived from calculations characterizing model systems. This Perspective describes the origins and uses of benchmarking and its applications in computational catalysis, heterogeneous catalysis, molecular catalysis, and electrocatalysis. It also discusses opportunities and challenges for future developments in these fields.

KEYWORDS: benchmarking, catalytic performance, computational catalysis, heterogeneous catalysis, molecular catalysis, electrocatalysis



Topics in Catalysis (2020) 63:1683–1699
<https://doi.org/10.1007/s11244-020-01380-2>

ORIGINAL PAPER



Towards Experimental Handbooks in Catalysis

Annette Trunschke¹ · Giulia Bellini¹ · Maxime Boniface¹ · Spencer J. Carey¹ · Jinhu Dong¹ · Ezgi Erdem^{1,2} · Lucas Foppa³ · Wiebke Frandsen¹ · Michael Geske² · Luca M. Ghiringhelli³ · Frank Girgsdies¹ · Rania Hanna¹ · Maike Hashagen¹ · Michael Hävecker^{1,4} · Gregory Huff¹ · Axel Knop-Gericke^{1,4} · Gregor Koch¹ · Peter Kraus¹ · Jutta Kröhnert¹ · Pierre Kube¹ · Stephen Lohr⁵ · Thomas Lunkenbein¹ · Liudmyla Masliuk¹ · Raoul Naumann d'Alnoncourt² · Toyin Omojola¹ · Christoph Pratsch¹ · Sven Richter¹ · Christian Rohner¹ · Frank Rosowski⁵ · Frederik Rütger² · Matthias Scheffler³ · Robert Schlögl^{1,4} · Andrey Tarasov¹ · Detre Teschner^{1,4} · Olaf Timpé¹ · Philipp Trunschke⁶ · Yuanqing Wang^{1,2} · Sabine Wrabetz¹

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Abstract

The “Seven Pillars” of oxidation catalysis proposed by Robert K. Grasselli represent an early example of phenomenological descriptors in the field of heterogeneous catalysis. Major advances in the theoretical description of catalytic reactions have been achieved in recent years and new catalysts are predicted today by using computational methods. To tackle the immense complexity of high-performance systems in reactions where selectivity is a major issue, analysis of scientific data by artificial intelligence and data science provides new opportunities for achieving improved understanding. Modern data analytics require data of highest quality and sufficient diversity. Existing data, however, frequently do not comply with these constraints. Therefore, new concepts of data generation and management are needed. Herein we present a basic approach in defining best practice procedures of measuring consistent data sets in heterogeneous catalysis using “handbooks”. Selective oxidation of short-chain alkanes over mixed metal oxide catalysts was selected as an example.

Northwestern
University

Currently in discussions that could lead to a larger collaboration:

Neil Schweitzer, Randy Snurr, Selim Alayoglu, Justin Notestein, Xijun Wang, Josh Kirkham

Reach out if you'd like to help us grow the database and this benchmarking effort!

Future updates: growing the database

- We plan to continue adding data from the literature



- We need your help – work with us and upload your results!



- May relax the peer-reviewed journal article requirement – what are your thoughts?

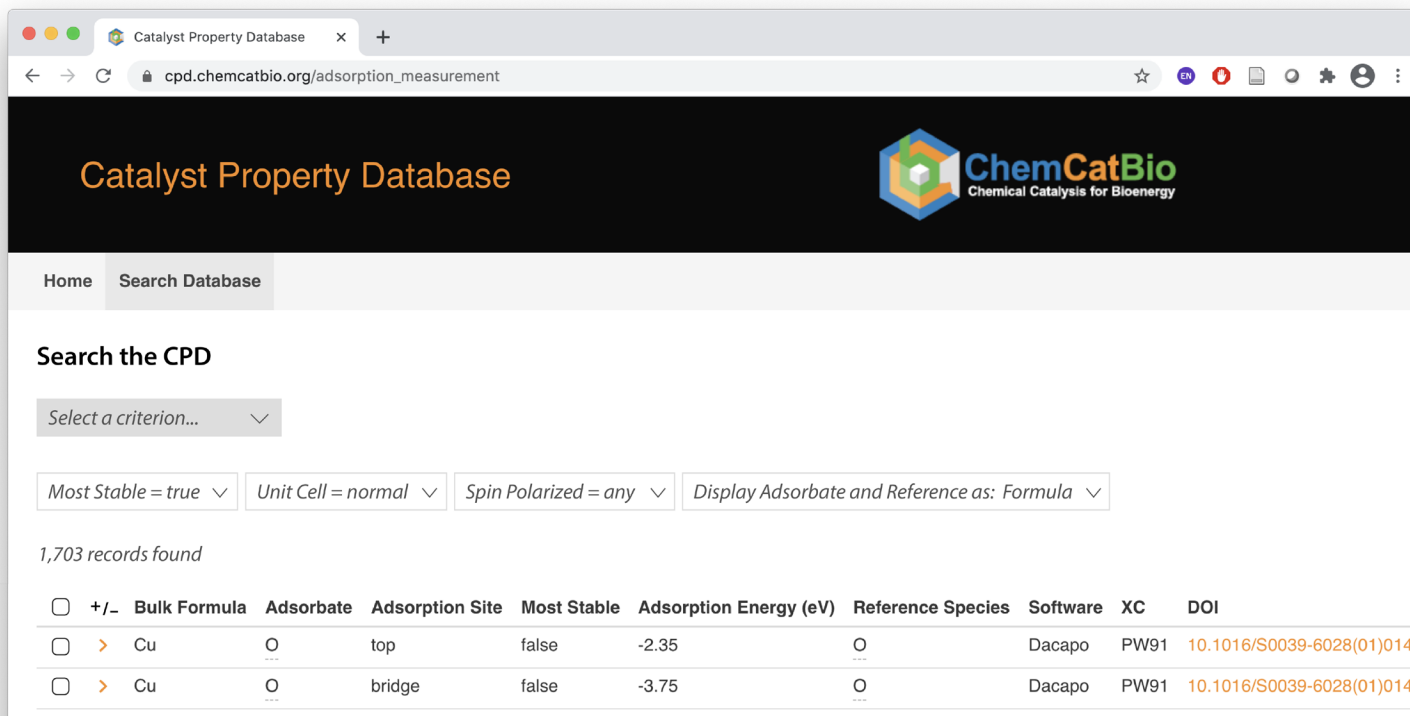
- Machine learning/natural language processing



Future updates: UI upgrades

Planned release this winter/spring

For example, adding pre-populated filters for the most common search preferences:



The screenshot shows a web browser window with the URL `cpd.chemcatbio.org/adsorption_measurement`. The page title is "Catalyst Property Database" and the ChemCatBio logo is visible. The search interface includes a "Search the CPD" section with a dropdown menu for "Select a criterion...". Below this, there are four pre-populated filter dropdowns: "Most Stable = true", "Unit Cell = normal", "Spin Polarized = any", and "Display Adsorbate and Reference as: Formula". The search results show "1,703 records found" and a table with columns: "+/-", "Bulk Formula", "Adsorbate", "Adsorption Site", "Most Stable", "Adsorption Energy (eV)", "Reference Species", "Software", "XC", and "DOI".

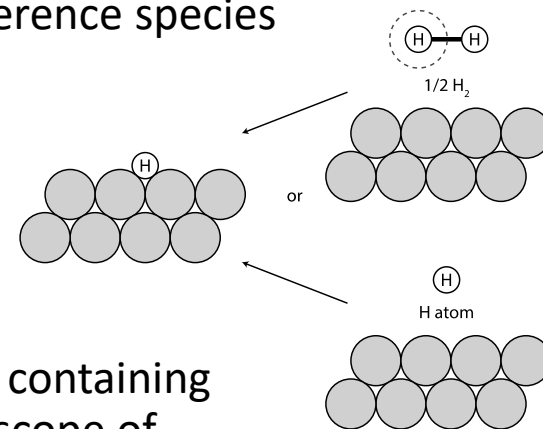
<input type="checkbox"/>	+/-	Bulk Formula	Adsorbate	Adsorption Site	Most Stable	Adsorption Energy (eV)	Reference Species	Software	XC	DOI
<input type="checkbox"/>	>	Cu	O	top	false	-2.35	O	Dacapo	PW91	10.1016/S0039-6028(01)0146
<input type="checkbox"/>	>	Cu	O	bridge	false	-3.75	O	Dacapo	PW91	10.1016/S0039-6028(01)0146

Future updates: Reference Species Translation

Background: Computed adsorption energies, the critical DFT output included in the Catalyst Property Database, may be reported with different reference species

Adsorption energy (E_{r}^* , in eV; 1 eV = 96.5 kJ/mol) for atomic H on a Pt(111) surface calculated with different gas-phase references.

Gas-phase reference	E_{r}^* (eV)	Difference (eV)
H	-2.80	2.26
$\frac{1}{2}\text{H}_2$	-0.54	



Problem: Data reported with different reference species, while containing similar information, **cannot be directly compared**, limiting the scope of data that can be applied in predictive catalyst applications

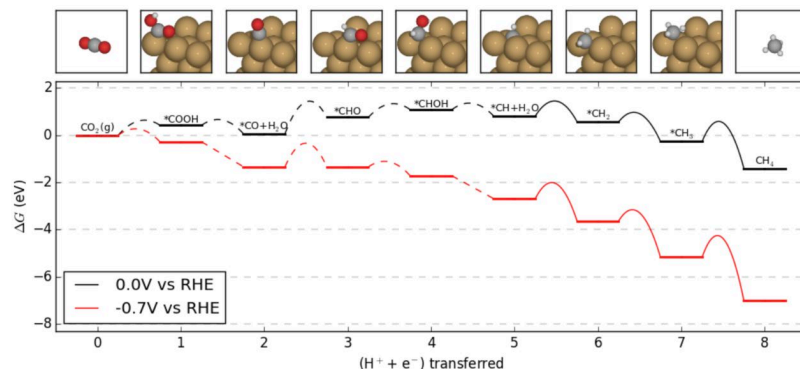
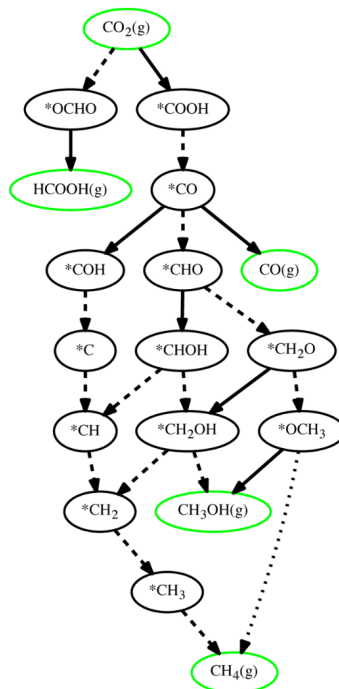
CPD Solution: Create a Reference Species Translation feature to enable interconversion between compatible reference species sets. Planned release next summer.

This is a key differentiator not found in any public database or resource.

Future updates: Reaction networks

Using the data generated for reference species translation, we could also generate reaction networks:

This would also allow us to cross-pollinate with databases containing reaction energies instead of adsorption energies, such as Catalysis Hub (SUNCAT)

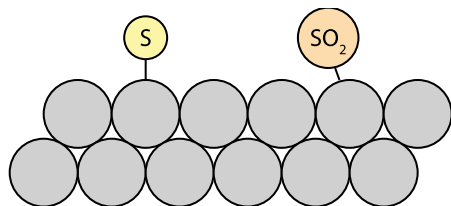


Figures from Norskov et al. *Org. Process Res. Dev.* **2016**, *20*, 1424–1430.

Future updates: Catalyst deactivation mitigation data

Create a catalyst deactivation mitigation resource in the CPD (release next fall)

- Adsorption energies for common catalyst poisons (alkali metals, halides, S, etc.) on common catalyst surfaces



Goal: enable researchers to make systematic predictions about catalyst deactivation rates

Future updates: more data types

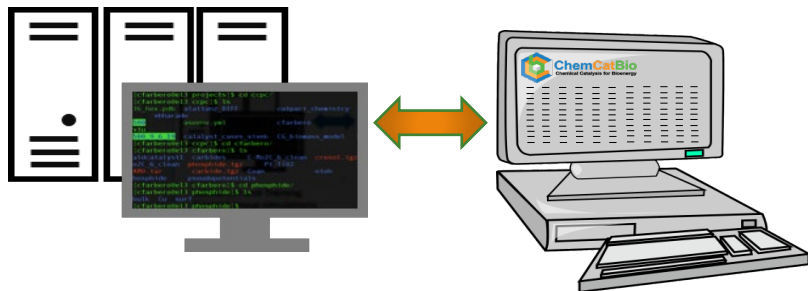
- Data types:**
- Computational catalysis (initial focus)
 - Catalyst characterization
 - Reaction performance

... we need your help with this!

Applications of the CPD

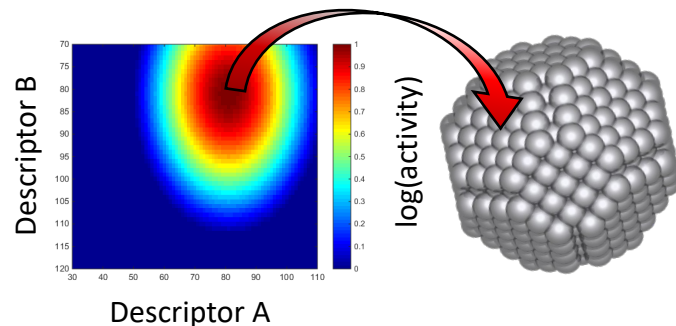
Benchmarking & Validation

Researchers wanting to check their results

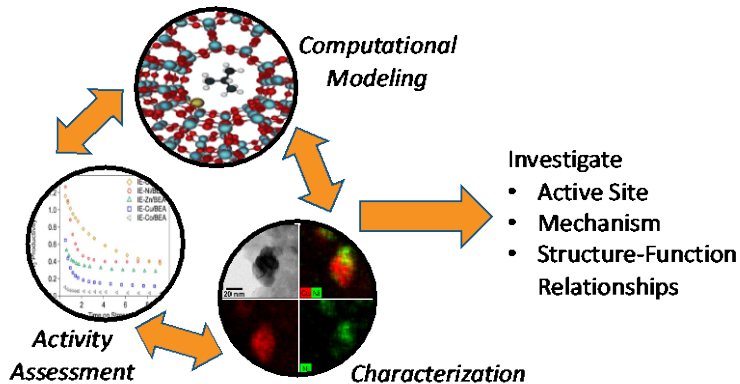


Catalyst Screening

Applying reactivity data to identify new target compositions

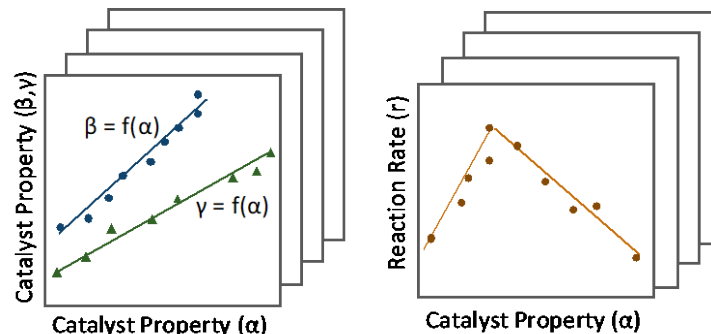


Interpretation of Experimental Trends



Discovery of Scaling Relations and Reactivity Descriptors

Harnessing the power of a large, central database



Acknowledgements

CHEM TEAM



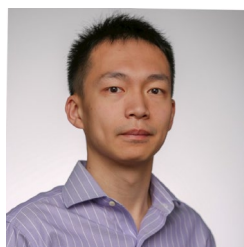
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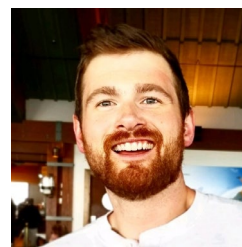
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Thank you. Let's Discuss.



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