

Center for  
**Programmable  
Energy Catalysis**

# Data Management in the Center for Programmable Energy Catalysis

Paul J. Dauenhauer (UMN)  
Director

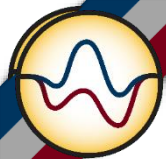
Susannah Scott (UCSB)  
Deputy Director



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

Funded by the U.S. Department of Energy, Office of Basic Energy Sciences

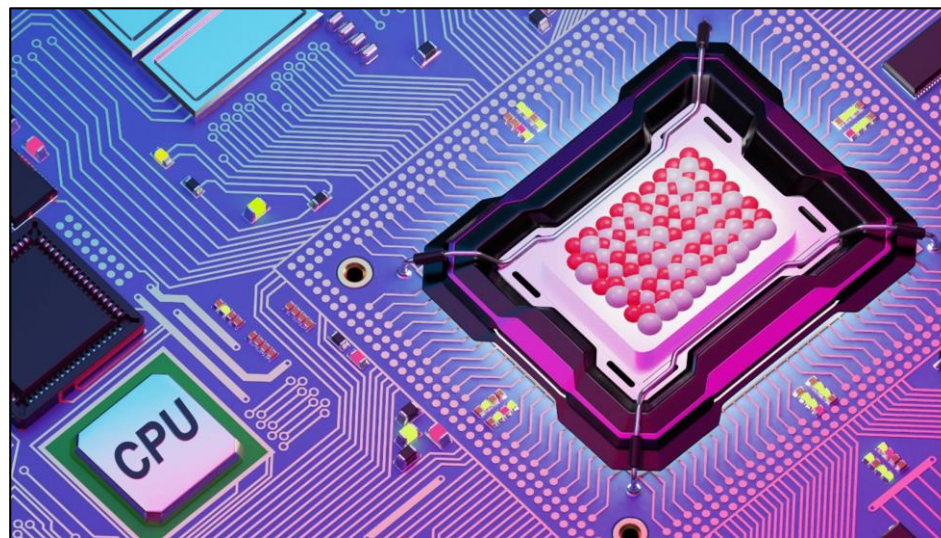


# Center for Programmable Energy Catalysis (CPEC)

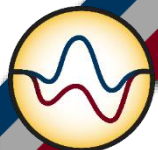
Inventing **tomorrow's advanced catalysts** through integration of chemical sciences

The DOE Center for Programmable Energy Catalysis (CPEC) **integrates expertise** in electronic materials, surface science, catalysis, and computational chemistry to invent and understand dynamic, programmable heterogeneous catalysts

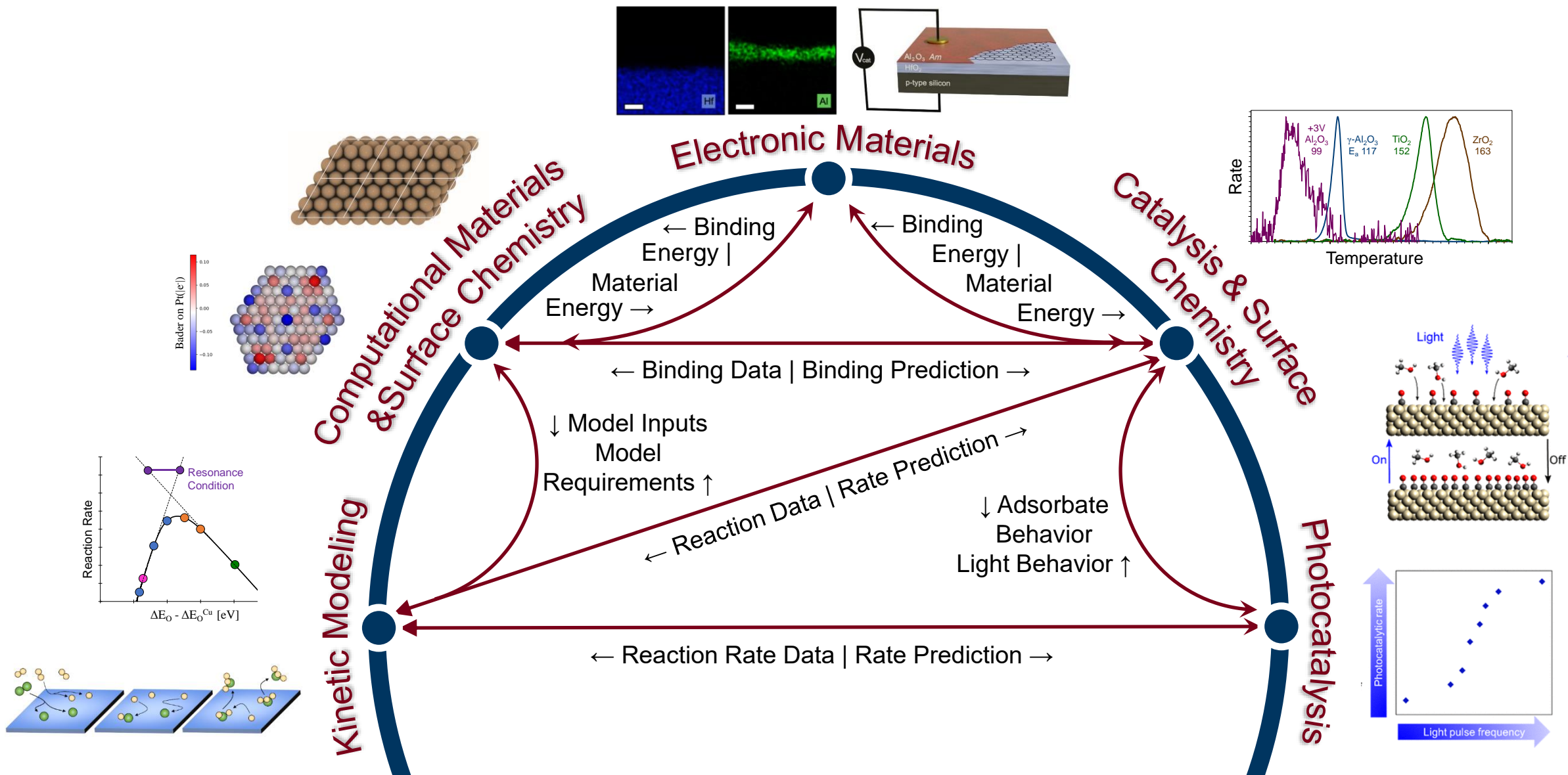
Programmable catalysts **change with time** at the frequency of surface reaction via a prescribed electronic 'program' that accelerates and controls reactions

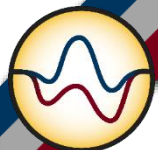






# How is CPEC multidisciplinary?





# CPEC: Unique Methods and Techniques → New Data

CPEC has created an array of new methods, tools, and techniques for fundamental research

Custom 1 cm<sup>2</sup> condenser reactor

Condenser cartridge holder

Isopotential titration (IPT)

In situ charge spectroscopy for condensers

- XPS / UPS, XAS

In situ reactor charge characterization

Scanning tunneling microscopy with charge

In situ IR reactor with charge application

Customized IR catalytic reactor

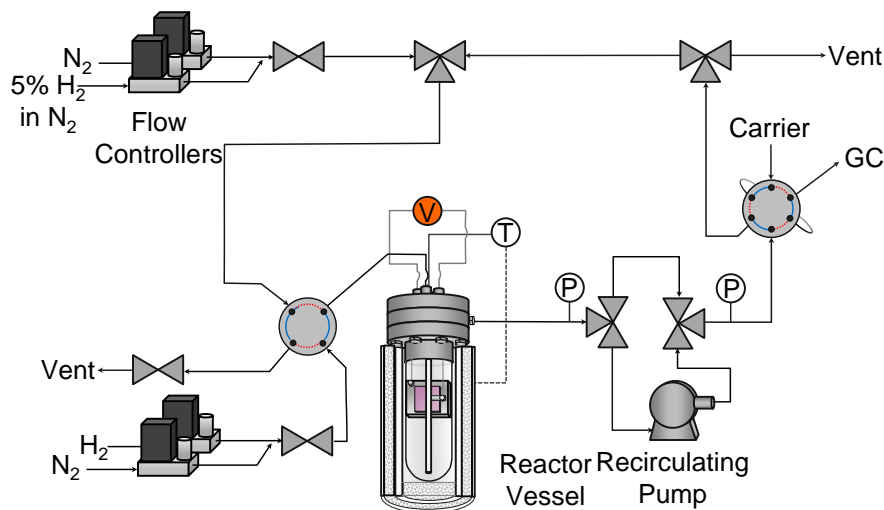
Transient IR reactor method

L<sup>3</sup> computational scaling for charge

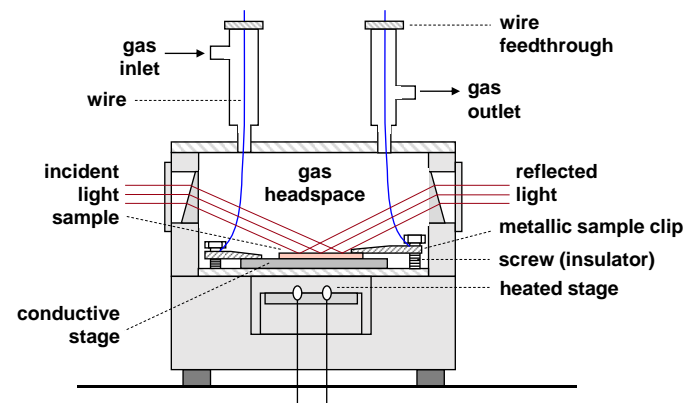
Dynamic microkinetic modeling

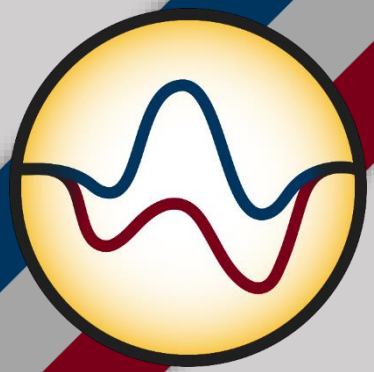
Dynamic kinetic Monte Carlo modeling

Bayesian optimization for dynamic reaction kinetic models



Pt/1 nm C/SiO<sub>2</sub>/Si

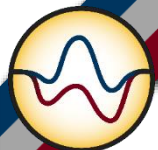




# **CPEC Data and Organization Policies**

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## **SHORT Term Data Sharing**



# Monthly Meetings - Required Attendance

**Monthly Team Meetings (each team)**  
**Quarterly Executive Committee Meetings**  
**Monthly All-Center Meetings**

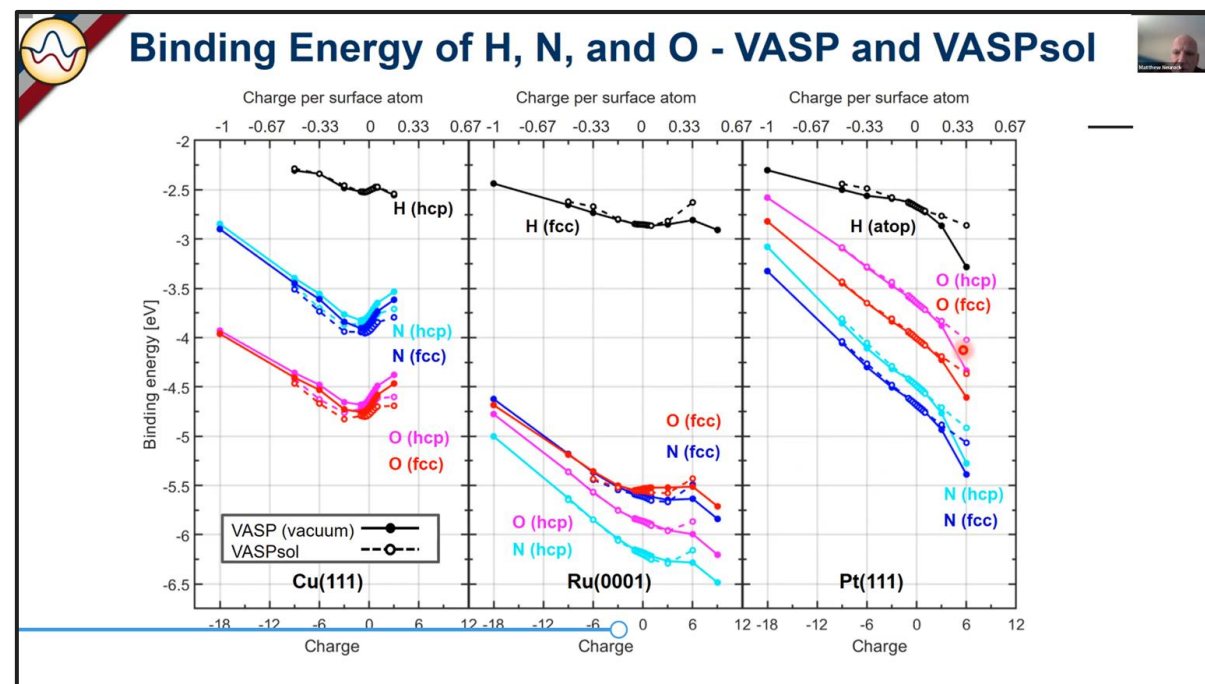
All researchers meet on zoom once per month: date organized by Magdalene

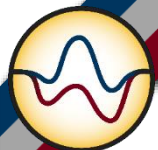
Start with confidentiality policy, safety spot discussion, and center updates

Technical content selected by Dauenhauer and Scott with input from executive committee

- Single CPEC PI presentation
- Two student talks (20 min each)
- External guest speakers

**CPEC All-Center Meeting**  
Zoom - December 2023  
Presenter: Prof. Matt Neurock





# CPEC Portal – Single place for all information


UNIVERSITY OF MINNESOTA  
Driven to Discover

A Department of Energy, Energy Frontier Research Center  
**Center for Programmable Energy Catalysis**

Mission Research Publications Team **Management** Support

## Management

The Center for Programmable Energy Catalysis (CPEC) provides online information for its members and partners through the secure CPEC portal at the link below.

 [Click here](#)

The shared portal information includes:

- Data Management Plan
- Presentation and Poster Templates

CPEC > CPEC\_Portal > Team\_01\_Carbon\_Condensers

Name ↑

- Conference Presentations
- Monthly Meetings
- Papers and Manuscripts
- Project Descriptions
- References



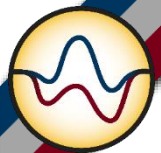
- A google document with links to different folders in google drive
- Each folder has different access permissions assigned by Dauenhauer or Miranda
- Some folders are read only; others are editable
- Content is updated as generated
- Recordings of meetings

## CPEC PORTAL

Center for Programmable Energy Catalysis

Access to the CPEC portal folders is controlled by Professor Paul Dauenhauer (hauer@umn.edu) and staff member, Magdalene Miranda (miran211@umn.edu). Please email them if you have trouble accessing any needed information.

1. [Policies](#)
2. [Templates](#) (Posters, Reports, Powerpoint, Logos)
3. [Member Information](#)
4. [Executive Committee](#)
5. [Team 01: Carbon Condensers](#)
6. [Team 02: Computation](#)
7. [Team 03: Dynamic Photocatalysis](#)
8. [Team 04: Nitrogen Condensers](#)
9. [Research Tools](#)
10. [Events](#)
11. [CPEC Advisory Board](#)
12. [Publications](#)
13. [Center Calendar](#)



# CPEC - Spring & Fall Annual Meetings

**Goal:** A combined research, training, education, and strategy session

**Mechanism:**

- Advisory board, faculty, and students fly to Minneapolis for a Friday + Saturday

**Content:**

- Workshop
- Poster sessions
- Discuss scientific progress
- Goals for next 6 months
- Advisory board meeting
- Open discussion & feedback
- Guest dinner speaker(s)



## Day 1 of 2

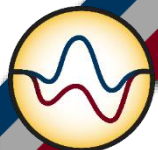
### CPEC SPRING MEETING

Friday, May 5, to Saturday, May 6, 2023

Location: Graduate Minneapolis Hotel, 615 Washington Ave. SE, Minneapolis, MN 55414

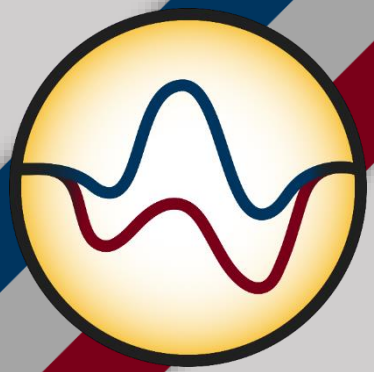
Friday, May 5 (All events in Graduate Hotel, Pinnacle Room & Foyer)		
Time (central)	Event/Topic	Speaker(s)
Before Noon	Arrive in Minneapolis (MSP Airport, Light Rail)	
Noon – 2:00 pm	Registration, Lunch, Hotel Check-in, Tours	
2:00 – 2:30	Introductions	Paul Dauenhauer Susannah Scott
2:30 – 3:30	Teams #1 & #4 – Catalytic Condensers	Lead: O. Abdelrahman
3:30 – 3:50	Coffee Break	
3:50 – 4:30	Programmable Catalysis Training Session (everyone)	Dauenhauer, Frisbie, Christopher
4:30 – 6:00	Poster Presentations + Coffee	
6:00 – 7:00	Dinner, Cash Bar	
7:00 – 8:00	Dessert + Cash Bar Featured Speakers Presentations (25+5 min each)	Tracy Lohr, Ph.D. Shell Javier Guzmann, Ph.D. ExxonMobil Chemical Company
8:00	Adjourn for the day	





# CPEC Portal – Single place for all information

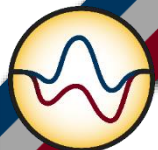
Center for Programmable Energy Catalysis									
Membership List & Contact Information									
Uni	Professor	Student / Post-Doc	Project #	Email	Phone	ORCID	Team	Member	Affiliate
	Staff: Becky Wyatt (Accountant)			huntx043@umn.edu	612/625-4071			X	
	Staff: Magdalene Miranda (General Manager)			miran210@umn.edu				X	
	Staff: Dan McDonald (Data & IT Manager)			mcdo0486@umn.edu				X	
<b>University of Minnesota</b>									
	Dauenhauer, Paul			hauer@umn.edu	612-343-5540	0000-0001-5810-1953	1,4	X	
		Gathmann, Sallye	1.1.1	gathm005@umn.edu			1	X	
		Onn, Tzia Ming	1.4.1	tonn@umn.edu			4	X	
		Hopkins, Justin	1.1.2	hopki361@umn.edu			1	X	
	Frisbie, Daniel			frisbie@umn.edu	612-516-9330	0000-0002-4735-2228	1,4	X	
		Student 1 (TBD)	1.1.3				1	X	
		Student 2 (TBD)	1.4.2				4	X	
	Bhan, Aditya			abhan@umn.edu	612-626-3981	0000-0002-6069-7626	1	X	
		First year student (To be c	1.1.3				1	X	
	Jalan, Bharat			bjalan@umn.edu			1,4	X	
		Shivasheesh Varshney	1.1.4	varsh022@umn.edu			1,4	X	
	Neurock, Matthew			mneurock@umn.edu			2	X	
		Kaida Liu	1.2.1	liu01485@umn.edu			2	X	



# **CPEC Data and Organization Policies**

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## **LONG Term Data Sharing**



# CPEC Data Management – Challenges & Policy

## Data sharing:

- To share machine-readable and digitally accessible data, including data that is published in charts and figures
- Transparency of post-processing
- Sharing more data than necessary, which could be useful to researchers inside and outside of CPEC, who can potentially re-use or re-interpret data that was inconclusive at the time

## Data preservation:

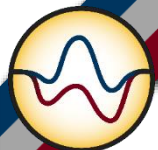
- To preserve data so that it can be used inside and outside of CPEC for years or decades to come

### Center for Programmable Energy Catalysis (CPEC) Data Management Plan

**Rationale.** The goal of the data management plan is to preserve and share the original research data acquired for the benefit of all participating members of the Center, DOE, and the public. To enable rapid and rigorous validation of our work by others, properly analyzed, pruned, and curated data will be rapidly shared through publication preferably in open access outlets or made available as freely available pre-print. Raw data sets will also be submitted to appropriate digital repositories that assign a digital object identifier (DOI) to the data sets. All mentioned data hosting services are for free, and no budget line items have been included.

**Data Collected, Generated, or Used.** All data generated in the Center are original and the investigators have the rights to share or otherwise manage data as described in this data management plan (DMP). Where commercial codes or copyrighted software packages are used (e.g. VASP, Gaussian) their proprietary source code, pseudopotentials, etc., cannot be shared, but are available to anyone who acquires the necessary software license from the vendor. We anticipate collecting, generating, or using the following types of original, publishable, and sharable data resulting from experiments, testing, synthesis, characterization, simulations, modeling, and machine-learning:

- **Raw Chromatographic/Spectroscopic Data:** Experimental data associated with reactivity measurements (GC, MS, FTIR, NMR) will be stored as raw data files in the format associated with commercial software used for each equipment. Similarly, catalyst characterization data using similar methods (Raman, FTIR, UV-vis, XRD, SEM, TEM, etc.) will be stored as raw data files in the format associated with software for each equipment. These files will be catalogued by experimental date, and a text file will be generated with the identical trial identification code containing the details related to the experimental conditions. Several gigabytes (GB) of this data type will be collected.
- **Raw Current – Voltage Data:** Experimental current-voltage measurements generated will be stored as Gamry files. These files will be catalogued by experimental date, and a text file will be generated with the identical trial identification code containing the details related to the experimental conditions. Several GB of this data type will be collected.
- **Interpreted Kinetic Data:** Calculations to interpret the raw information including calibration and kinetic rate calculations will be stored in excel files. Included in the file will be a description of the experiments for each data set. Several megabytes (MB) of this data type will be generated.
- **Processed images, photos, movies, videos, and micrographs:** Experimental setups and observations will be documented with photos or videos; final configurations of atomistic simulations will be rendered to image files and reaction pathways are visualized as short animations/videos; characterization includes various forms of microscopies (SEM, S/TEM) producing image files. The image/movie files will be used in publications or presentations. Image and video files will use several hundred GB.
- **Hand-written notebook entries:** Lab notebooks will be used to record details of experimental procedures, synthesis techniques, catalyst preparation, experimental measurements, and simulation strategies. Notebooks will have persistent unique identifiers, will be individually numbered, and each experiment will have a title, date, and summary. Notebooks will be kept in a secure location in each Investigator's lab.
- **Electronic lab notebooks:** Detailed description of all modeling studies and notes about computational setups will be stored in electronic lab notebooks or appended to the dissertation/thesis of all students involved with the project.
- **Electronic structure calculation results:** The file types will include atomic position files, startup/run files, simulation output files, Python scripts used for data analysis and automation, novel programs developed for specialized data analysis, and program output files from data analysis programs. Raw data for all these file types will likely exceed 2 TBs, and many simulation output files will be greater



# CPEC Data Management – Sharing Strategy

Primary focus is on making data available via publication and associated methods  
**Part 1: Promote preprints and ensure publications are openly available**

Include data sets within the supporting information files

We provide the OSTI to all  
CPEC publications on our  
website

Center for Programmable Energy Catalysis ChemRxiv™

**Title of Your Preprint Goes Here for All to Read**

Author<sup>1,2</sup>, Author<sup>1,2</sup>, Author<sup>2</sup>, Author<sup>3</sup>, Author<sup>2</sup>, Author<sup>4</sup>, Author<sup>5</sup>, Author<sup>1,2</sup>, Author<sup>1,3</sup>, Author<sup>2</sup>, Author<sup>1,4</sup>, Author<sup>1,2</sup>, CorrespondingAuthor<sup>1,2\*</sup>

<sup>1</sup> Center for Programmable Energy Catalysis (CPEC), University of Minnesota, 421 Washington Ave. SE, Minneapolis, MN, USA 55455.  
<sup>2</sup> University of Minnesota, Department of Chemical Engineering & Materials Science, 421 Washington Ave. SE, Minneapolis, MN, USA 55455  
<sup>3</sup> William A. Brookshire Department of Chemical and Biomolecular Engineering and Texas Center for Superconductivity (TcSUH), University of Houston, Houston, TX, USA, 77204  
<sup>4</sup> Department of Chemical Engineering, University Massachusetts Amherst, 686 N. Pleasant Street, Amherst, MA, USA, 01003  
<sup>5</sup> Characterization Facility, University of Minnesota, 100 Union Street SE, Minneapolis, MN, 55455, USA  
\* Corresponding author: hauer@umn.edu

**Abstract.** Accelerating catalytic chemistry and tuning surface reactions requires precise control of the electron density of metal atoms. In this work, nanoclusters of platinum were supported on a graphene sheet within a catalytic condenser device that facilitated electron or hole accumulation in the platinum active sites with negative or positive applied potential, respectively. The catalytic condenser was fabricated by depositing on top of a p-type Si wafer an amorphous HfO<sub>2</sub> dielectric (70 nm), on which was placed the active layer of 2–4 nm platinum nanoclusters on graphene. Potential of  $\pm 6$  V applied to the Pt/graphene layer relative to the silicon electrode moved electrons into or out of the active sites of Pt, attaining charge densities more than 1% of an electron or hole per surface Pt atom. At a level of charge condensation of 1–10% of an electron per surface atom, the binding energy of carbon monoxide to a Pt(111) surface was computed via density functional theory to vary from 5 to 48 kJ mol<sup>-1</sup> (0.05–0.50 eV), which was consistent with the range of carbon monoxide binding energies determined from temperature programmed desorption ( $\Delta BE_{CO}$  of 20±1 kJ mol<sup>-1</sup> or 0.19 eV) and equilibrium surface coverage measurements ( $\Delta BE_{CO}$  of 14±1 kJ mol<sup>-1</sup> or 0.14 eV). Impedance spectroscopy indicated that Pt/graphene condensers with potentials oscillating at 3,000 Hz exhibited negligible loss in capacitance and charge accumulation, enabling programmable surface conditions at amplitudes and frequencies necessary to achieve catalytic resonance.

**1.0 Introduction.** The emergence of cost-competitive solar and wind power in the past decade has transformed the landscape for renewable energy economics and applications.<sup>[1,2]</sup> Produced in rural locations frequently far from industrial and urban centers, the challenge remains to store renewable energy for on-demand use across daily and seasonal requirements.<sup>[3]</sup> Batteries, compressed air, and pumped water storage are potentially viable options for local electrical storage, but they remain stationary preferably near the location of energy generation.<sup>[4,5]</sup> Alternatively, conversion of renewable electrical power to

baseload power provided by conventional fossil-fuel-derived power and high rates of renewable energy implementation.<sup>[6]</sup>

**2.0 Results and Discussion.** Programmable catalysis is a proposed design strategy capable of accelerating catalytic reaction rates above the Sabatier limit for a given reaction<sup>[8]</sup> and selectively pushing reactions away from equilibrium via work input directly to the catalytic surface.<sup>[23]</sup> The properties of inorganic catalysts are typically invariant with time (with the exceptions of restructuring and deactivation), therefore,

JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY pub.acs.org/JACS Article

**Platinum Graphene Catalytic Condenser for Millisecond Programmable Metal Surfaces**

Tzia Ming Omn, Sallye R. Gathmann, Silu Guo, Surya Pratap S. Solanki, Amber Walton, Benjamin J. Page, Geoffrey Rojas, Matthew Neurock, Lars C. Grabow, K. Andre Mkhoyan, Omar A. Abdelrahman, C. Daniel Frisbie, and Paul J. Dauenhauer\*

Cite This: *J. Am. Chem. Soc.* 2022, 144, 22113–22127 Read Online

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**ABSTRACT:** Accelerating catalytic chemistry and tuning surface reactions require precise control of the electron density of metal atoms. In this work, nanoclusters of platinum were supported on a graphene sheet within a catalytic condenser device that facilitated electron or hole accumulation in the platinum active sites with negative or positive applied potential, respectively. The catalytic condenser was fabricated by depositing on top of a p-type Si wafer an amorphous HfO<sub>2</sub> dielectric (70 nm), on which was placed the active layer of 2–4 nm platinum nanoclusters on graphene. A potential of  $\pm 6$  V applied to the Pt/graphene layer relative to the silicon electrode moved electrons into or out of the active sites of Pt, attaining charge densities more than 1% of an electron or hole per surface Pt atom. At a level of charge condensation of  $\pm 10\%$  of an electron per surface atom, the binding energy of carbon monoxide to a Pt(111) surface was computed via density functional theory to change 24 kJ mol<sup>-1</sup> (0.25 eV), which was consistent with the range of carbon monoxide binding energies determined from temperature-programmed desorption ( $\Delta BE_{CO}$  of 20  $\pm$  1 kJ mol<sup>-1</sup> or 0.19 eV) and equilibrium surface coverage measurements ( $\Delta BE_{CO}$  of 14  $\pm$  1 kJ mol<sup>-1</sup> or 0.14 eV). Impedance spectroscopy indicated that Pt/graphene condensers with potentials oscillating at 3000 Hz exhibited negligible loss in capacitance and charge accumulation, enabling programmable surface conditions at amplitudes and frequencies necessary to achieve catalytic resonance.

**INTRODUCTION**

Over the past century, metal surfaces have been synthesized for precise electronic interaction with adsorbates to accelerate reactions and control catalytic pathways.<sup>1–7</sup> Bulk metals were converted to nanoclusters supported on metal oxides and carbon surfaces, providing higher dispersion and increased densities of edge, step, and terrace sites.<sup>8–11</sup> These active metal surfaces were further refined by alloying with other metals,<sup>12</sup> adding promoters and inhibitors that further modify their properties,<sup>13</sup> and designing the catalyst/support interactions.<sup>14,15</sup> Precise synthesis of more advanced nanoparticles and surface design included core-shell particles,<sup>16,17</sup> intermetallic surfaces,<sup>18,19</sup> and single-atom alloys<sup>16,17,20</sup> to provide more electronic specification at the active site by altering the coordination of the atoms and the composition of nearest neighbors.<sup>21</sup> Such synthetic methods, however, require precise surface structures in stable conformations and only provide discrete options for active sites that are static on the time scale of the catalytic turnover.

An alternative approach to catalyst design directly tunes the electron density of the active site by stabilizing positive or negative charge in the exposed catalytic surface.<sup>14,22</sup> We

recently described the method of a 'catalytic condenser' that uses a high- $\epsilon$  dielectric HfO<sub>2</sub> layer to separate a conductive silicon electrode from a conductive active layer of ultrathin amorphous alumina on graphene.<sup>23</sup> In this example, the amorphous alumina layer is a solid Lewis acid catalyst, while the supporting graphene rapidly distributes charge across the device surface. When a positive voltage bias is applied to the active alumina/graphene layer relative to the silicon electrode, the alumina catalyst active sites are depleted of electrons, making them more acidic and faster at dehydrating alcohols such as isopropyl alcohol.

Synthesizing the catalytic condenser stack design with a metal-on-graphene active layer (instead of an oxide on graphene) extends condenser applicability to many important metal-catalyzed chemistries. However, electronically biasing

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DOE STI Management System**

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For awards made on or after October 1, 2014, submission to DOE of accepted manuscripts is being required (see [DOE STIP Public Access FAQs](#)). Even if not specifically required under your award, you may submit an accepted manuscript of a journal article for work published as a result of DOE funding via AN 241.3 or the new AM Submission Interface for inclusion in DOE PAGES.

Submission Options for Financial Assistance Recipients (Grantees)

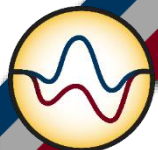
Final Technical Report, Accepted Manuscript of Journal Article, or other STI Product (AN 241.3) Submission Interface

SBIR/STTR Certification

Scientific Research Datasets (AN 241.6) Submission Interface

A few important tips...  
Set your browser to accept all cookies before starting the submission process.





# CPEC Data Management – Sharing *Strategy*

Primary focus is on making data available via publication and associated methods

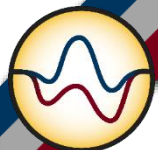
## Part 2: Require code & data set sharing with prescribed methods

Simulation Codes: CPEC Github Site

The screenshot shows the Github profile for the Center for Programmable Energy Catalysis. The profile includes a logo, a bio, and a list of repositories. The 'Popular repositories' section highlights a repository named 'ProgrammableOER', which is a public fork of 'srgathmann/ProgrammableOER'. The repository description states: 'Code accompanying "Dynamic Promotion of the Oxygen Evolution Reaction via Programmable Metal Oxides" by S. R. Gathmann, et al. (ChemRxiv 2024)'. It is identified as a 'Jupyter Notebook'.

Large Data Sets: CPEC Data Conservancy

The screenshot shows the University Digital Conservancy page for a dataset. The page is titled 'Data for: Catalytic Resonance Theory: Negative Dynamic Surfaces for Programmable Catalysts'. It includes a breadcrumb trail: 'Home > Open Scholarship and Data > Data Repository for U of M (DRUM) > Data for: Catalytic Resonance Theory: Negative Dynamic Surfaces for Programmable Catalysts'. The dataset is attributed to 'Gathmann, Sallye R; Ardagh, M Alexander; Dauenhauer, Paul J (2021-08-14)'. A thumbnail image shows a schematic of catalytic surfaces with labels 'A' and 'B'. The page provides a 'Published Date' of 2021-08-14 and lists the authors: 'Gathmann, Sallye R', 'Ardagh, M Alexander', and 'Dauenhauer, Paul J'. It also includes a 'Persistent link to this item' with two URLs: 'https://doi.org/10.13020/vwy0-gs56' and 'https://hdl.handle.net/11299/223076'. The 'Group' is identified as 'Dauenhauer Group'. The 'Author Contact' is 'Dauenhauer, Paul J' with the email 'hauer@umn.edu'. The 'Keywords' are 'energy', 'catalysis', and 'storage'. The 'Type' is 'Dataset'.

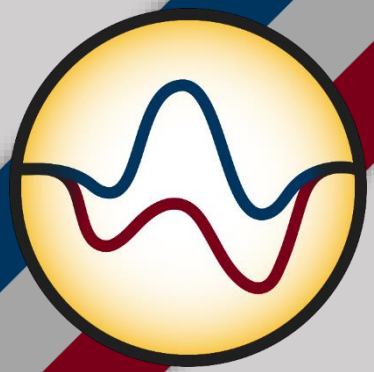


# CPEC Data Management – Sharing Strategy

Primary focus is on making data available via publication and associated methods

## Part 3: Review and compliance via data tracking within the Portal

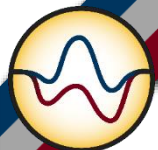
	A	B	C	F	G	H	I	J	K	L	M	
1												We
2		Paper #	Title	Preprint?	OSTI	Peer Reviewed	Accepted?	Publication Year	Journal	DOI#	Journal IF (2022)	S
3		P024	Epitaxially Grown Single-Crystalline SrTiO <sub>3</sub> Membranes using a Solution-Processed, amorphous SrCa <sub>2</sub> Al <sub>2</sub> O <sub>6</sub> Sacrif	No	2430017	Yes	Yes	2024	Journal of Materials Chemistry	10.1039/D4TC02030H		
4		P023	Catalytic Resonance Theory: Forecasting the Flow of Programmable Catalytic Loops	Yes	TBD	Yes						
5		P022	ATLAS-MAP: An Automated Test Station for Gated Electronic Transport Measurements	Yes	2439068	Yes	Yes	2024	ACS Measurement Science Au			
6		P021	Catalytic Resonance Theory: The Catalytic Mechanics of Programmable Ratchets	Yes	2407234	Yes	Yes	2024	Chemical Science	10.1039/D4SC04069D		
7		P020	Alumina-Titania Nanolaminate Condensers for Hot Programmable Catalysis	Yes	2377755	Yes	Yes	2024	ACS Materials Letters	10.1021/acsmaterialslett.4c00652		
8		P019	Anomalous frequency and temperature dependent scattering in the dilute metallic phase in lightly doped SrTiO <sub>3</sub>	Yes	2427951	Yes	Yes	2024	Physical Review Letters	arXiv:2402.18767		
9		P018	Isopotential Titration for Quantifying Metal-Adsorbate Charge Transfer	Yes	TBD	Yes						
10		P017	CatTestHub: A Benchmarking Database of Experimental Heterogeneous Catalysis for Evaluating Advanced Materials	Yes	TBD	Yes						
11		P016	Accelerated Steam Methane Reforming by Dynamically Applied Charges	Yes	TBD	Yes	Yes	2024	Journal of Physical Chemistry	10.1021/acs.jpcc.4c01311		
12		P015	Dynamic Promotion of the Oxygen Evolution Reaction via Programmable Metal Oxides	Yes	2335550	Yes	Yes	2024	ACS Energy Letters	10.1021/acsenergylet	22	
13		P014	Bond Selective Photochemistry at Metal Nanoparticle Surfaces: CO Desorption from Pt and Pd	No	2350681	Yes	Yes	2024	JACS Journal of the American	10.1021/jacs.3c13874	15	
14		P013	Is There a Discernible Photochemical Effect Beyond Heating for Visible Photon-Mediated NH <sub>3</sub> Decomposition over Ru/	No	2337785	Yes	Yes	2024	Journal of Physical Chemistry	10.1021/acs.jpcc.4c0	3.7	
15		P012	Deciphering the Olefin Isomerization-Polymerization Paradox of Palladium(II) Diimine Catalysts: Discovery of Simultan	No	2267576	Yes	Yes	2023	Journal of the American Chem	10.1021/jacs.3c01513	15	
16		P011	Hybrid Molecular Beam Epitaxy for Single-Crystalline Oxide Membranes with Binary Oxide Sacrificial Layers	Yes	2283938	Yes	Yes	2024	ACS Nano	10.1021/acsnano.3c1	17.1	
17		P010	Up Up Down Down Left Right Left Right B A Start for the Catalytic Hackers of Programmable Materials	Yes	2228578	Yes	Yes	2023	Matter	10.1016/j.matt.2023.1	19.8	
18		P009	Catalytic Resonance Theory: Circumfluence of Programmable Catalytic Loops	Yes	2290247	Yes	Yes	2024	Journal of Catalysis	10.1016/j.jcat.2024.11	7.3	
19		P008	Flexible and Extensive Platinum Ion Gel Condensers for Programmable Catalysis	Yes	2263306	Yes	Yes	2024	ACS Nano	10.1021/acsnano.3c0	17.1	
20		P007	Fabrication of Large Area Metal-on-Carbon Catalytic Condensers for Programmable Catalysis	Yes	2263446	Yes	Yes	2023	ACS Applied Materials & Interf	10.1021/acsam.3c14	9.5	
21		P006	Programmable Catalysis by Support Polarization: Elucidating and Breaking Scaling Relations	Yes	2222558	Yes	Yes	2023	Nature Communications	10.1038/s41467-023-	16.6	
22		P005	Energy Flows in Static and Programmable Catalysts	Yes	1971068	Yes	Yes	2023	ACS Energy Letters	10.1021/acsenergylet	22	
23		P004	Writing the Programs of Programmable Catalysis	Yes	1971823	Yes	Yes	2023	ACS Catalysis	10.1021/acscatal.3c0	12.9	
24		P003	Sn-modified BaTiO <sub>3</sub> thin film with enhanced polarization	No	1924658	Yes	Yes	2023	Journal of Vacuum Science &	10.1116/6.0002208	2.6	
25		P002	Overcoming the Entropy Penalty of Direct Air Capture for Efficient Gigatonne Removal of Carbon Dioxide	Yes	1914328	Yes	Yes	2023	ACS Engineering Au	10.1021/acsengineeri	NA	
26		P001	Platinum Graphene Catalytic Condenser for Millisecond Programmable Metal Surfaces	Yes	1899709	Yes	Yes	2022	Journal of the American Chem	10.1021/jacs.2c0948	15	
27												



# **CPEC Data and Organization Policies**

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**CURATED Data Sharing - CatTestHub**



# Curated Data: CatTestHub

## Parameters relevant to reactor type

- Reactor configuration
- Reactor ID linking to a reactor description page

## Parameters relevant to fluid phase

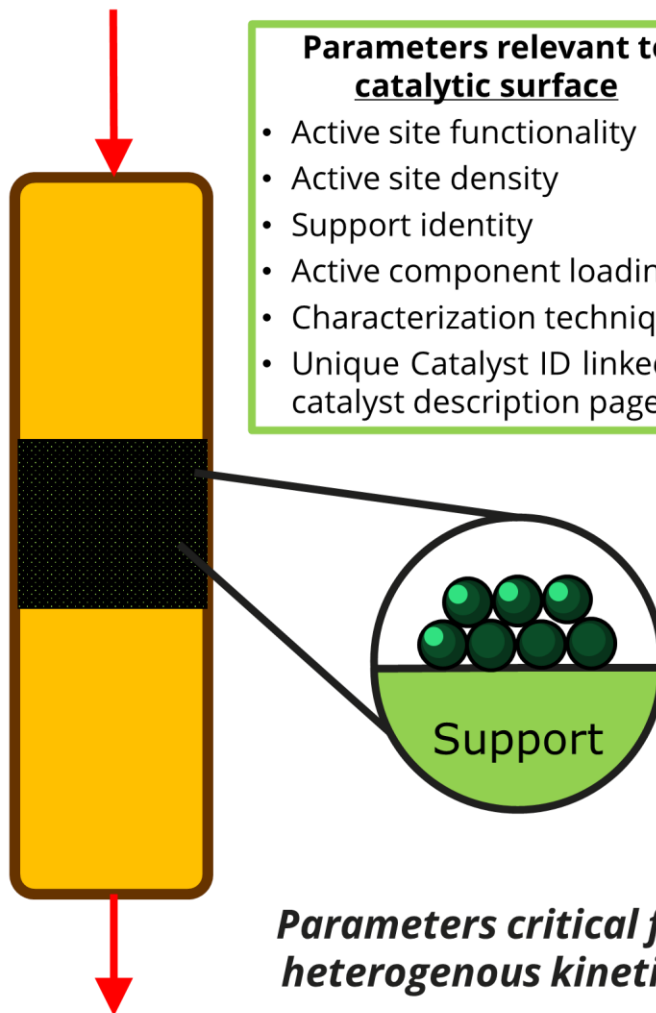
- Reaction Conditions – Pressure/ Temperature
- Feed Chemical Composition
- Total molar flow rate

## Parameters relevant to catalytic bed

- Pellet Diameter
- Space Velocity

## Parameters relevant to observable macroscopic quantities

- *Apparent* rate of catalytic turnover
- Product Selectivity
- Reactant conversion
- Atom/Mole Balance



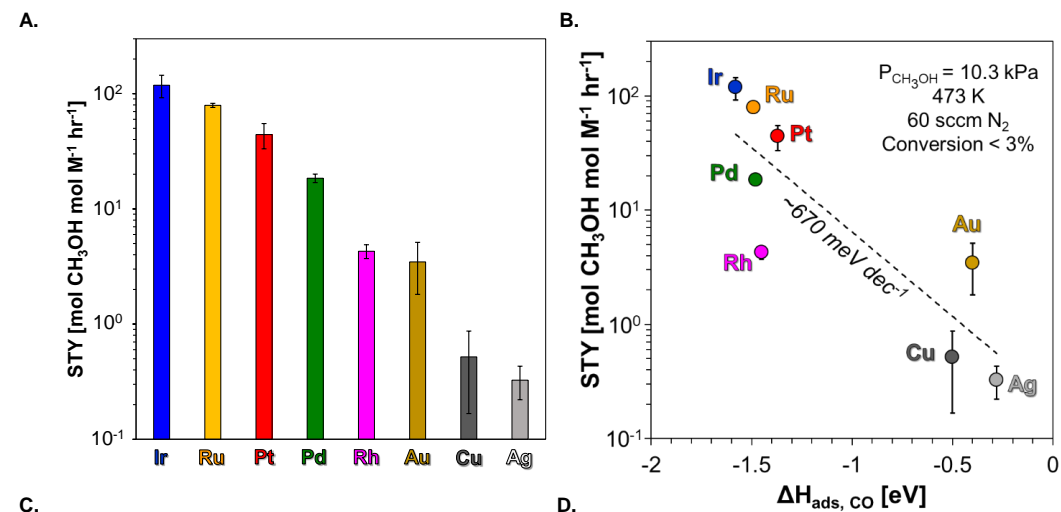
## Parameters relevant to catalytic surface

- Active site functionality
- Active site density
- Support identity
- Active component loading
- Characterization techniques
- Unique Catalyst ID linked to catalyst description page

*Parameters critical for heterogenous kinetics*

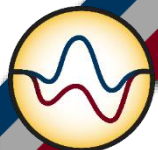
## Goals:

- (1) Create a high quality data set for comparison with dynamic kinetics
- (2) Capture all relevant experimental and characteristic data



Methanol Dehydrogenation






# Curated Data: CatTestHub

UNIVERSITY OF MINNESOTA  
Driven to Discover


A Department of Energy, Energy Frontier Research Center  
**Center for Programmable Energy Catalysis**

Mission Research Publications Team Management Support **CatTestHub** Media



## CatTestHub


An open database of experimental catalysis data



**ENTER THE DATABASE**


The CPEC Chemical Catalysis Database is a collection of experimental chemical information over catalytic surfaces. The CPEC chemical catalysis database was designed to house experimentally measured kinetic, thermodynamic, and characterization information relevant to chemical turnover on catalytic surfaces. Within the database, you can select from a growing list of catalytic chemistries that have been experimentally measured by CPEC members or curated from the scientific literature.

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## CatTestHub

An open database of experimental catalysis data

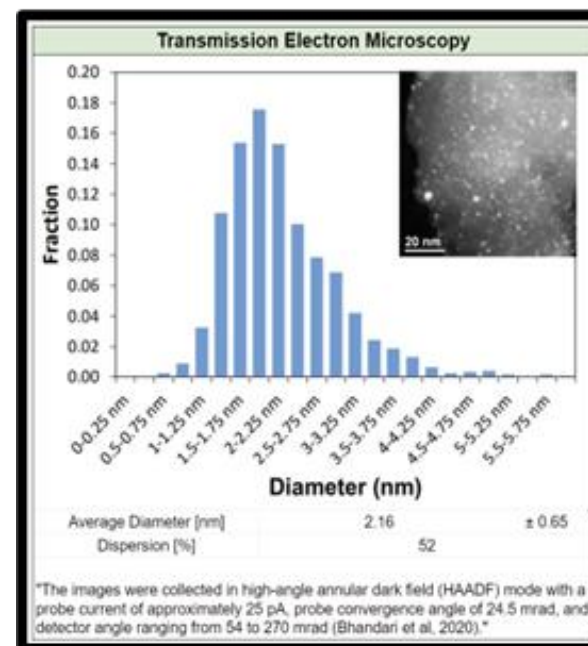
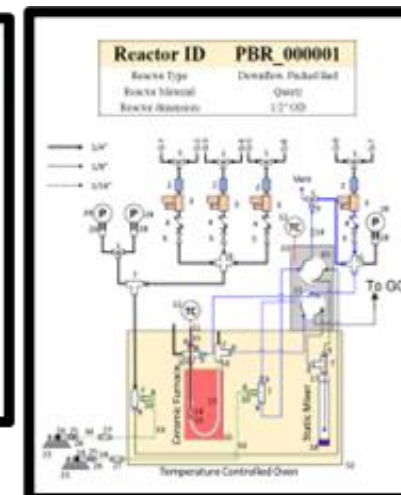


Welcome to the CPEC Chemical Catalysis Database (CatTestHub) - A collection of experimental chemical information over catalytic surfaces. The CPEC chemical catalysis database was designed to house experimentally measured kinetic, thermodynamic, and characterization information relevant to chemical turnover on catalytic surfaces. Below you can select from a growing list of catalytic chemistries that have been experimentally measured by CPEC members or curated from the scientific literature.

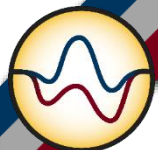
**Catalytic Chemistry** — Begin by selecting a chemistry link

- Methanol Dehydrogenation
- Hofmann Elimination
- Formic Acid Decomposition

The CPEC Chemical Catalysis Database was developed as part of benchmarking efforts by members of the Center for Programmable Energy Catalysis, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences (WDE-SC0023464).



Metal Catalysts			
Metal	Support	Loading	Description
Platinum	Silica	1	<a href="#">Cat_M_000001</a>
Platinum	Silica	3.1	<a href="#">Cat_M_000002</a>
Iridium	Carbon	1	<a href="#">Cat_M_000003</a>
Platinum	Silica	1	<a href="#">Cat_M_000004</a>
Platinum	Carbon	5	<a href="#">Cat_M_000005</a>
Palladium	Carbon	5	<a href="#">Cat_M_000006</a>
Ruthenium	Carbon	5	<a href="#">Cat_M_000007</a>
Rhodium	Carbon	5	<a href="#">Cat_M_000008</a>
Gold	Carbon	5	<a href="#">Cat_M_000009</a>
Silver	Carbon	5	<a href="#">Cat_M_000010</a>
Platinum	Carbon	1	<a href="#">Cat_M_000011</a>
Copper	Carbon	5	<a href="#">Cat_M_000012</a>
Palladium	Carbon	1	<a href="#">Cat_M_000013</a>
Gold	Silica carbide	1	<a href="#">Cat_M_000014</a>
Nickel	Carbon	5	<a href="#">Cat_M_000015</a>



# Structure – People – Teams – Executive Committee

## Leaders



★ Director  
Paul  
Dauenhauer



★ Deputy  
Director  
Susannah  
Scott



Managing  
Director  
Magdalene  
Miranda



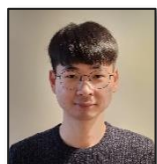
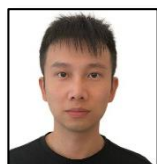
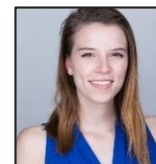
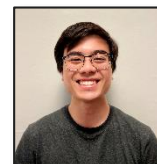
Accountant  
Stephanie  
Pederson



Executive  
Committee

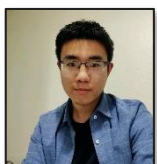
## Team 1

Lead Omar  
Abdelrahman



## Team 2

Lead Rachel  
Getman



## Team 3

Lead Phil  
Christopher

