

## ChemCatBio Webinar Series

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



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Chemical Catalysis for Bioenergy Consortium

Wednesday, October 13, 2021

12–12:45 p.m. MDT

Webinar Link and Registration:

<https://nrel.webex.com/nrel/onstage/g.php?MTID=eff19fe27734bae3349285008c713838c>

The ChemCatBio Data Hub project aims to accelerate catalyst research by developing transformational tools. In September 2020, the project released the [Catalyst Property Database](#) (CPD), a free and public resource. The CPD was designed in response to the observation that when data—such as computed reaction energetics—is used in catalyst design, it is almost always generated by the researchers seeking to use it, even if similar data has been published previously. One barrier to data reuse that results in this duplication of effort is the difficult process of finding and applying published data, which can be slow, error-prone, and manual. The CPD seeks to overcome these challenges by creating a centralized, searchable database of quality catalyst property data. By making published catalyst data much easier to find and apply, we aim to enable benchmarking and advanced data science applications in catalysis while reducing duplication of effort. At present, the CPD focuses on computed adsorption energies for intermediates on catalytic surfaces gathered from peer-reviewed journal articles. The database is uniquely suited to catalyst development in biomass conversion, as it was designed specifically to handle complex adsorbates such as those found in biomass vapor streams. These features also make it useful in a wide range of chemical transformations.

In this webinar, we will share the motivations for the CPD, how to search and upload data, applications, and future plans to grow types and quantity of data.

For more information, please visit our website at [ChemCatBio.org](https://ChemCatBio.org) or email us directly at [Contact@ChemCatBio.org](mailto:Contact@ChemCatBio.org). ChemCatBio is funded by the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) Bioenergy Technologies Office.