CKineticsDB: An Extensible and FAIR Datahub for Multiscale Modeling in Heterogeneous Catalysis

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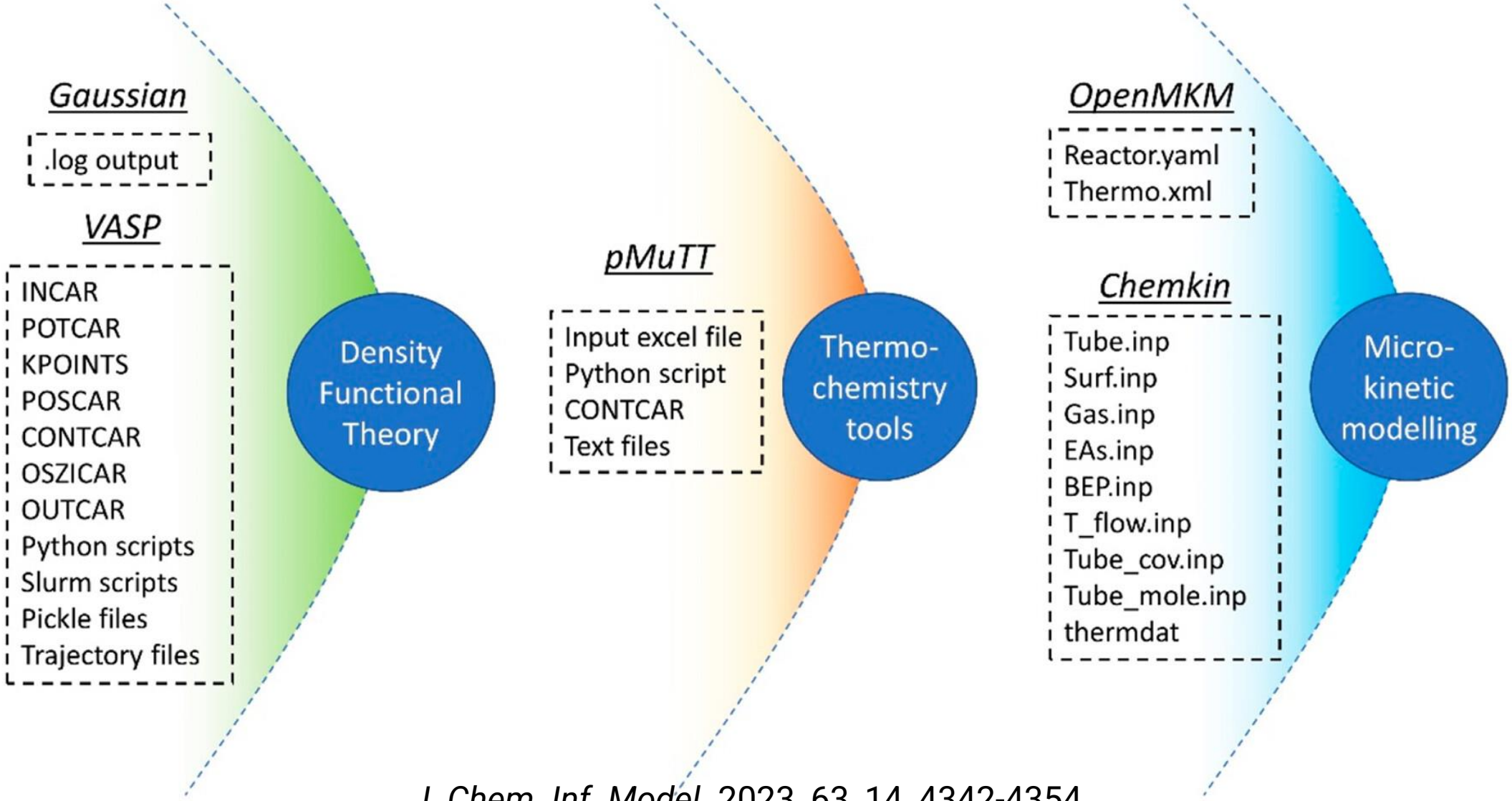
CKineticsDB: An Extensible and **FAIR**[1] Datahub for Multiscale Modeling in Heterogeneous Catalysis

Findable, Accessible, Interoperable, Reusable

- Easily share and integrate data
- Make data interpretable by humans and by machines

1. Wilkinson, M. D. et. al. Comment: The FAIR Guiding Principles for scientific data management and stewardship. Sci. Data 2016, 3, 160018

CKineticsDB stores the simulation files involved in multiscale modeling



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Chemical Kinetics Database

Multiscale Modeling in Catalysis

Microkinetic Modeling
Thermochemistry
Density Functional Theory

Unaltered files

Organize

Categorize

Curate

Extract Metadata

Store files, metadata, quality test results

Microkinetic models, species- and reaction-specific simulations, and other output based on requested metadata

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CKineticsDB top-level components

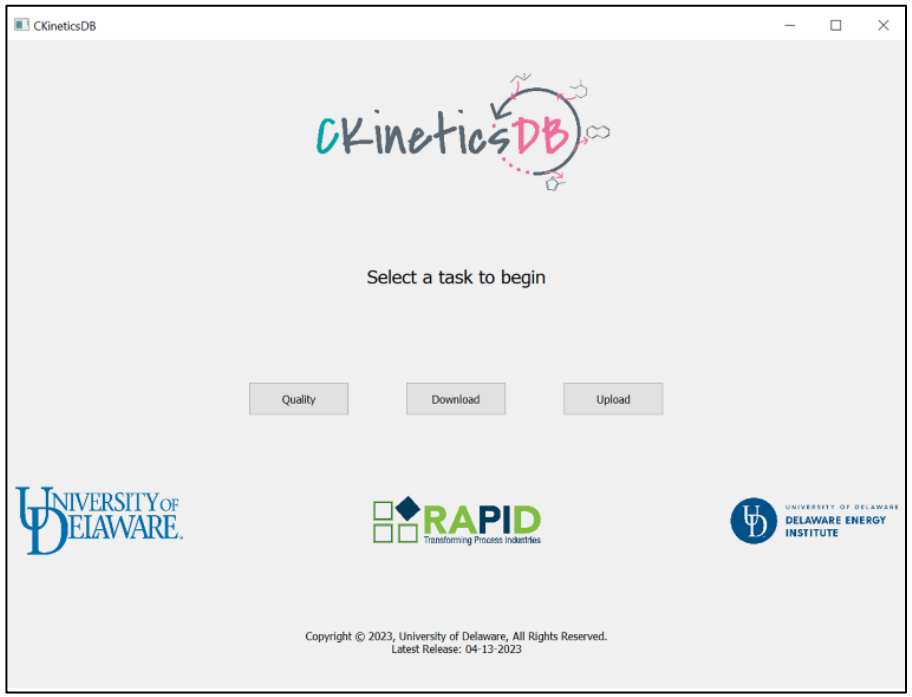
Database Management System

MongoDB is a, non-relational, document-oriented database

Frontend Python Software

Enables integrations with Vlachos Group in-house tools

Graphical User Interface



Command line interface

```
$ ckineticsdb download [OPTIONS]
$ ckineticsdb upload [OPTIONS]
$ ckineticsdb quality [OPTIONS]
```

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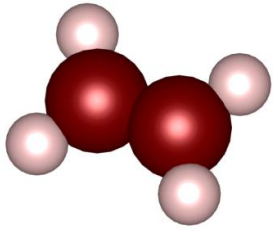
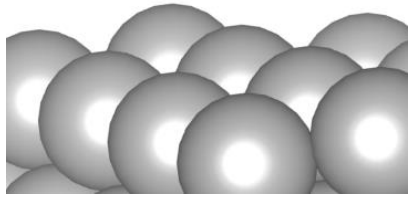
Current data snapshot

14000+ DFT calculations

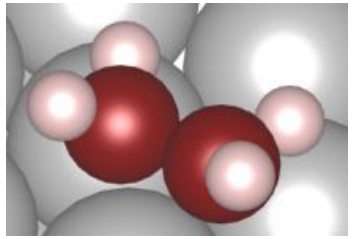
Gas Phase



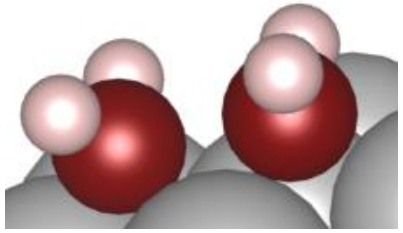
Bulk structures



Adsorbates



Transition states



Catalysts

Pure Metals
Ag, Au, Cu, Ir, Ni,
Pd, Pt, Rh, Ru

Zeolites
H-BEA

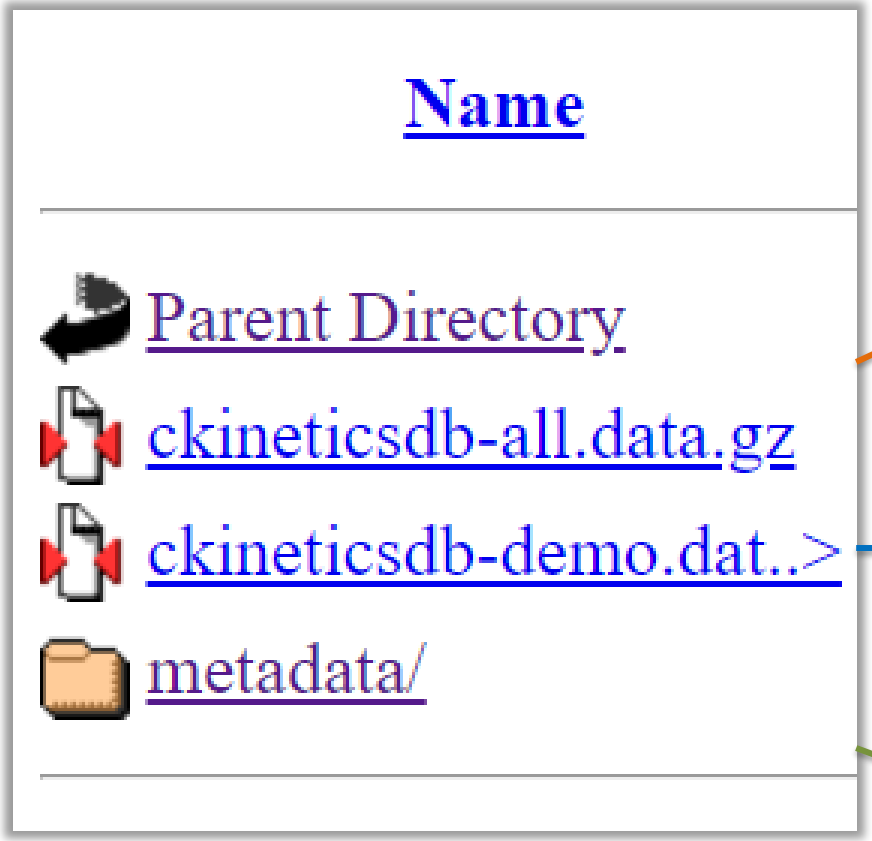
Metal oxides
Al_2O_3, ReO_x, TiO_2,
SiO_2, ZrO_2

Reaction Chemistries

Hydrogenolysis, dehydrogenation, hydroformylation, hydrodeoxygenation, C-O bond activation, and acylation; several catalyst facets and active center structures

CKineticsDB data is openly shared online

Available at: https://files.ccei.udel.edu/p/CKineticsDB/data/



Data associated with several publications of Vlachos group pertaining to microkinetic modeling

Demo containing only one dataset to test software setup

MS Excel and JSON files containing metadata of the complete dataset available above

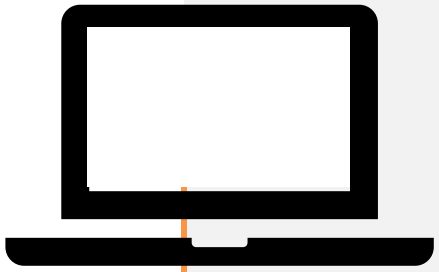
CKineticsDB Data Workflow

https://files.ccei.udel.edu/p/CKineticsDB/data/

Compressed data snapshots generated by MongoDB

Download dataset

User

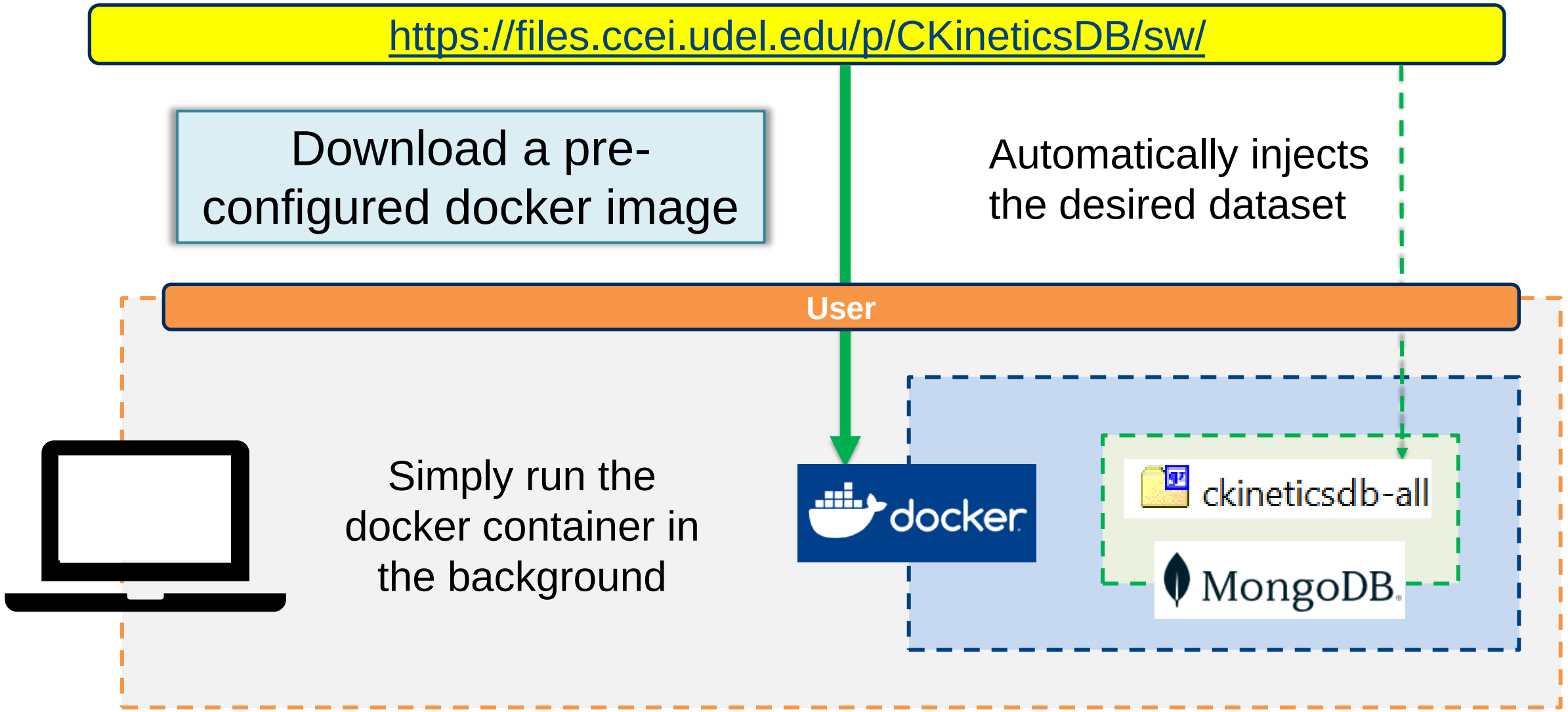


Run a MongoDB instance and unpack data

MongoDB.

ckineticsdb-all

CKineticsDB Data Workflow

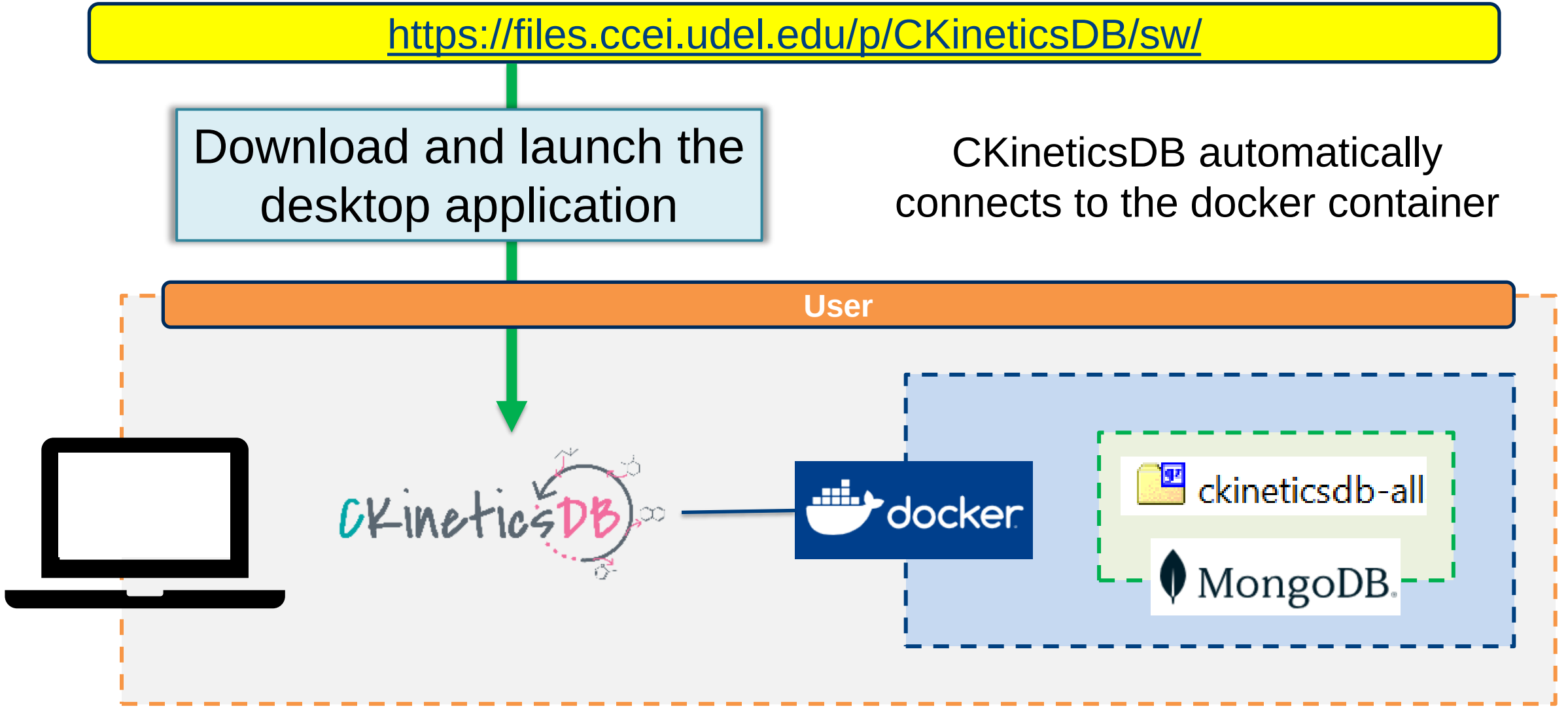


CKineticsDB Data Workflow

https://files.ccei.udel.edu/p/CKineticsDB/sw/

Download and launch the desktop application

CKineticsDB automatically connects to the docker container



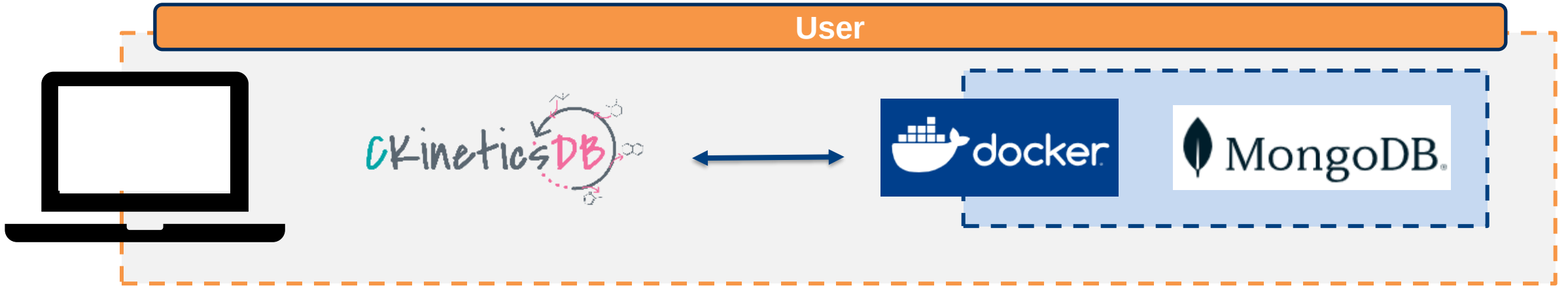
Download CKineticsDB as a desktop application separate from the data

University of Delaware HPC

https://files.ccei.udel.edu/p/CKineticsDB/

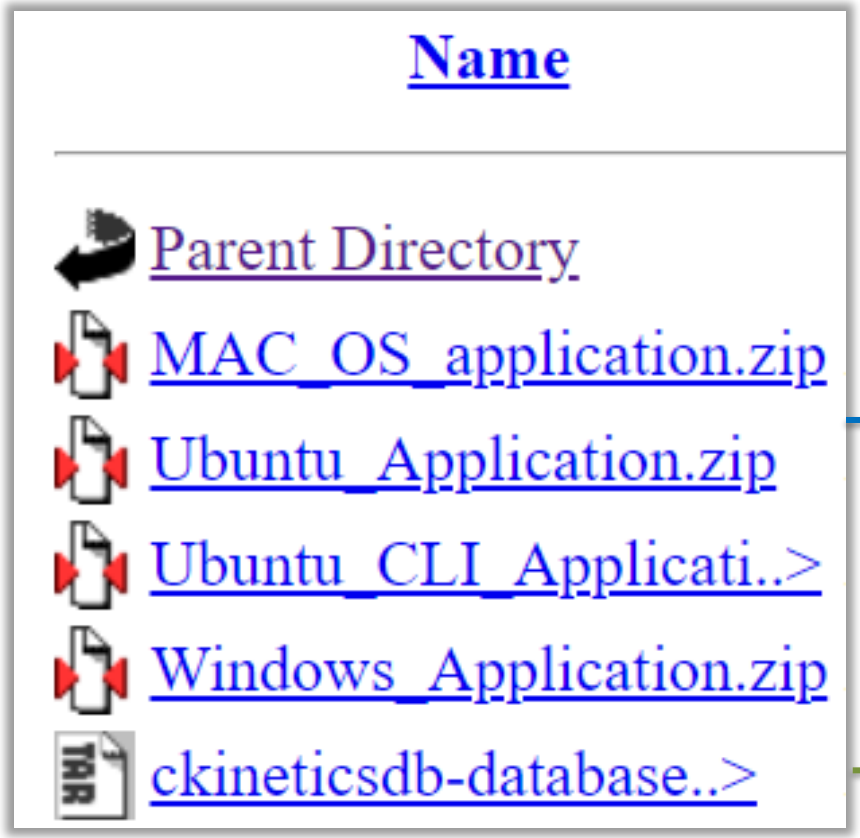
Users don't need to -
- Learn MongoDB
- Run a local database server
- Worry about data persistence

Users can -
- Connect CKineticsDB to any different database, local or remote
- Use CKineticsDB with their local data



CKineticsDB Software Components

Available at: https://files.ccei.udel.edu/p/CKineticsDB/sw/



Get access credentials by emailing to vkineticslab@udel.edu

Application.zip:
- Desktop application executable
- MongoDB server credentials file
- Template files and readMe file

-ckineticsdb-database.tar: Pre-configured docker image

Getting Started – Setting up the database

Detailed documentation at: https://github.com/VlachosGroup/ckineticsdb-documentation

1. Install Docker Desktop (from Docker website)

2.1. Download and load the Docker image:

Load the image: `> docker load --input <path_to>/ckineticsdb-database.tar`

2.2. Run a docker container and specify the data snapshot of choice to be injected

Options to inject different data snapshots – Default option

Running the container with no specific options will download and inject the demo data snapshot by default

ckineticsdb-demo.

```
>>> docker run --name ckineticsdb-db -p 27017:27017 ckineticsdb-database:latest
```

Add a URL: Download and inject a specific data snapshot from the website

Add a local path: Inject a downloaded data snapshot locally

Syntax for each option is available in documentation

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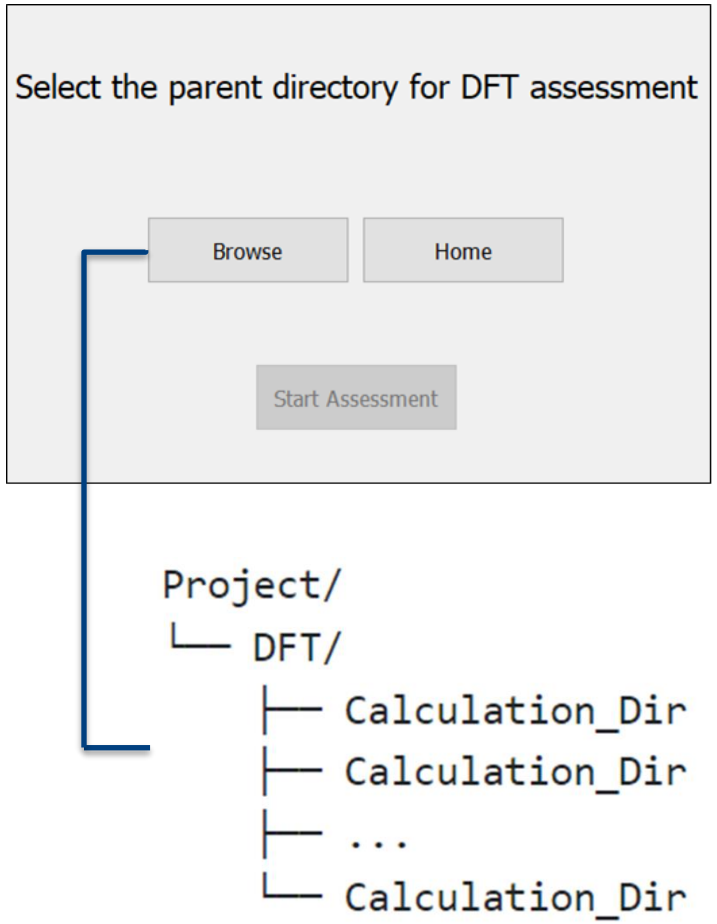
Demo

- Graphical user interface
- Parameters to browse and make selections in the GUI for downloading data

DFT data quality assessment

Select the directory of calculations to be tested



Identify the type of calculation ------ Relaxation, Dimer, NEB, etc.

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Run tests based on the calculation ----- Convergence, KPOINTS, more

↓

Provide results and a dataset summary

Assessment results (PDF)

Missing files (MS Excel)

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DFT Data Quality Tests and Output

Software	Calculation	Quality Test(s)
VASP	Ionic Relaxation	Convergence, Kpoints, Encut
VASP	Dimer	Convergence, Curvature, Kpoints, Encut
VASP	(Climbing - /) Nudged Elastic Band (inclusive of all images)	Convergence of the highest energy image, Kpoints, Encut
VASP	Individual NEB Image	Convergence
VASP	Frequency Analysis	Frequencies assessment, Kpoints, Encut
Gaussian	Optimization	Convergence
Gaussian	Frequency Analysis	Frequencies assessment

Summary of a complete dataset's assessment

Summary:

Total Number of Calculations: 239

Passed all tests: 168

Need to be reviewed: 71

Related Inconsistencies:

Ionic step information not available : 4

More than one imaginary frequencies : 10

No frequencies found in vibrational calculation : 56

No POSCAR file : 1

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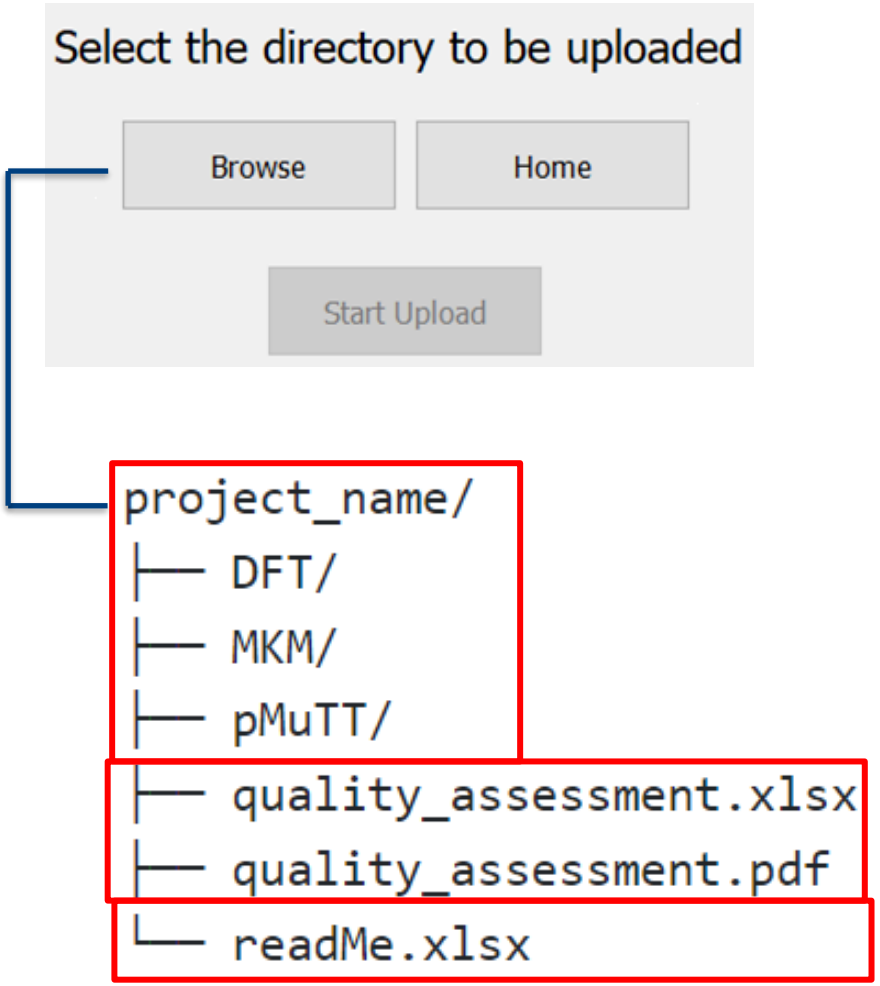
Demo

- Data Quality Assessment Results

Conditions to upload a new dataset to CKineticsDB



Organize the files as per the Data Organization Policy

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Run data quality assessment and include results

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Complete the readMe.xlsx file with materials information, software information, and other required details

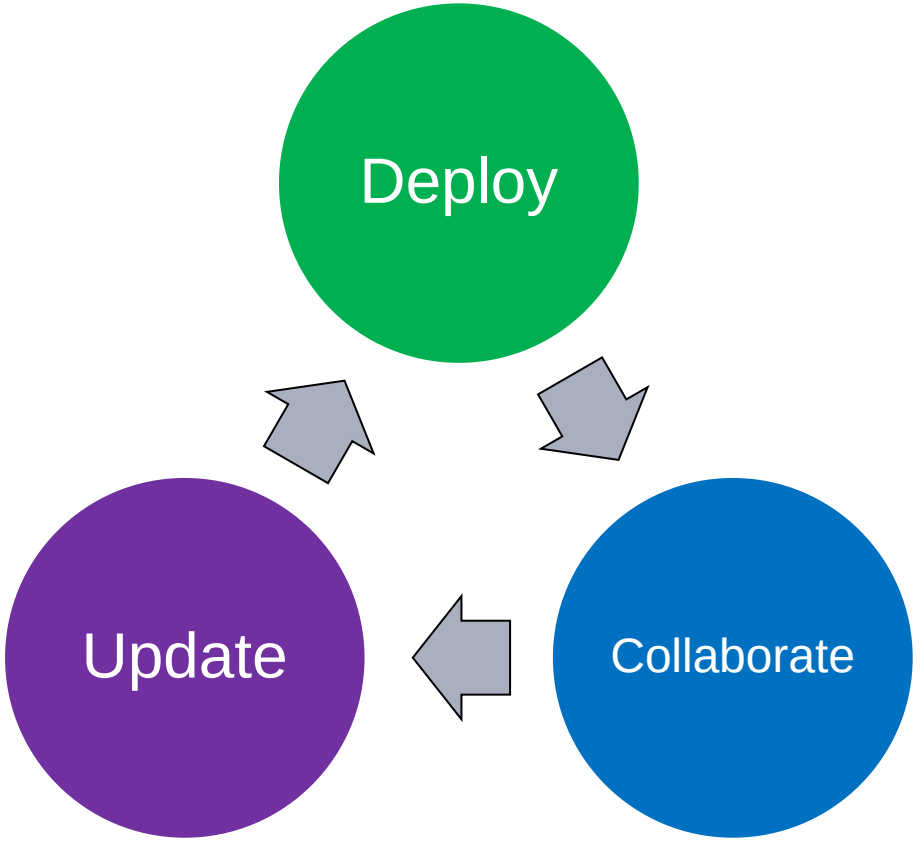
↓

Upload

Value in data management for multiscale modeling in catalysis

Organize Data	Extract Information	Accelerate applications
Reaction Data	• Reaction mechanisms, microkinetic models • Kinetic and thermochemical parameters	• Minimize DFT simulations • Facilitate thermodynamic and kinetic studies • Utilize chemically similar data for new mechanisms • Develop multiscale software
Thermochemistry	• Scripts to process DFT output; data from NIST • DFT energies and frequencies	
DFT calculations of molecules	• Input settings • Catalyst specifications	

Collaboration and Future Development



- Update CKineticsDB for common needs of groups
- Cover more simulation software
- Build new data-based features
- Guide Onboarding

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CKineticsDB

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CKineticsDB Paper: https://doi.org/10.1021/acs.jcim.3c00123

Thank you

Documentation: https://github.com/VlachosGroup/ckineticsdb-documentation

CKineticsDB