Applications of the ASE database
calculational workflows and data sharing

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U.S. DEPARTMENT OF ENERGY
Office of Science
SLAC NATIONAL ACCELERATOR LABORATORY

Why do we need databases?

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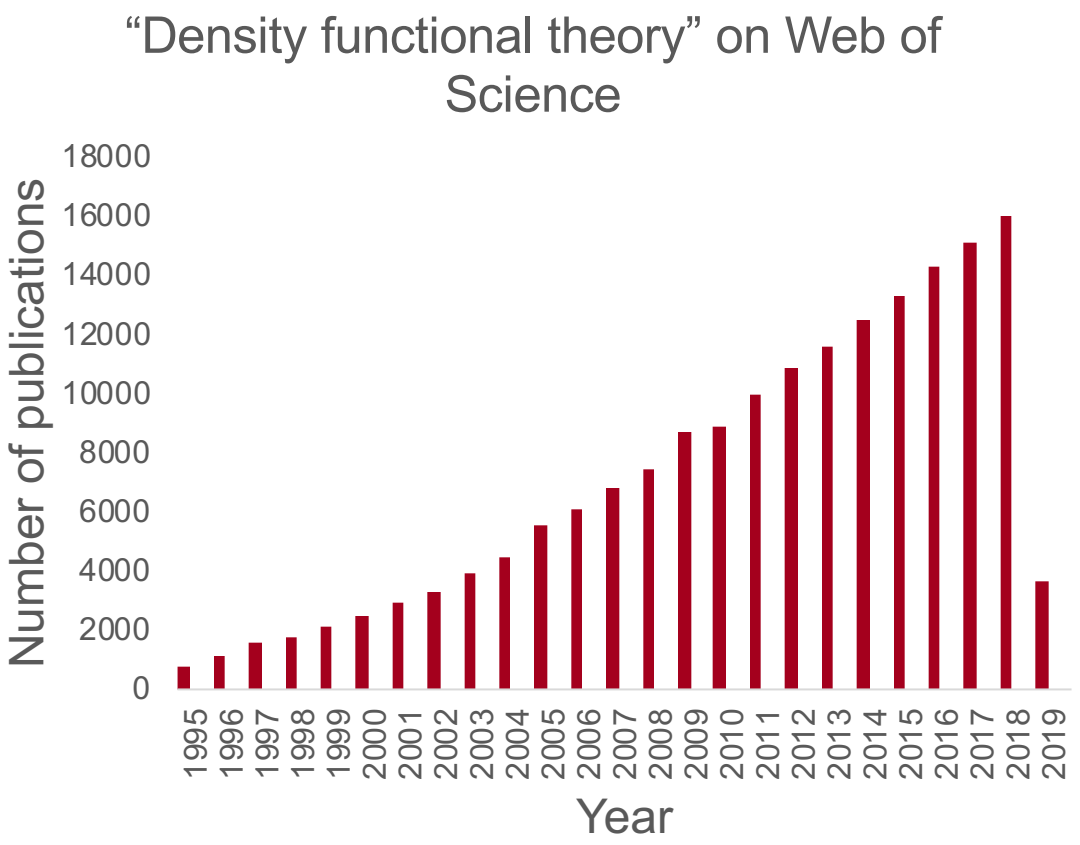
- Sharing and handling increasing amount of DFT data.



NOMAD

OQMD

MATERIALSCLOUD

The Materials Project
materialsproject.org

AFLOW
Automatic - FLOW for Materials Discovery

Outline

- Introduction to the ASE database.
- Application of the database
  - Local handling of atomic structures and calculations
  - Server side open databases – catalysis-hub.org
  - Machine learning workflows

- Suggested improvements and future plans.

Overview of the ASE database implementation:

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J.J. Mortensen

David Kleiven

SQL?

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- ASE uses Structured Query Language (SQL)
  - Data is organized in well-defined tables.
  - Commands to efficiently select, write, update or delete.

```
sqlite > SELECT * FROM systems WHERE energy < -10 AND fmax < 0.01;
```

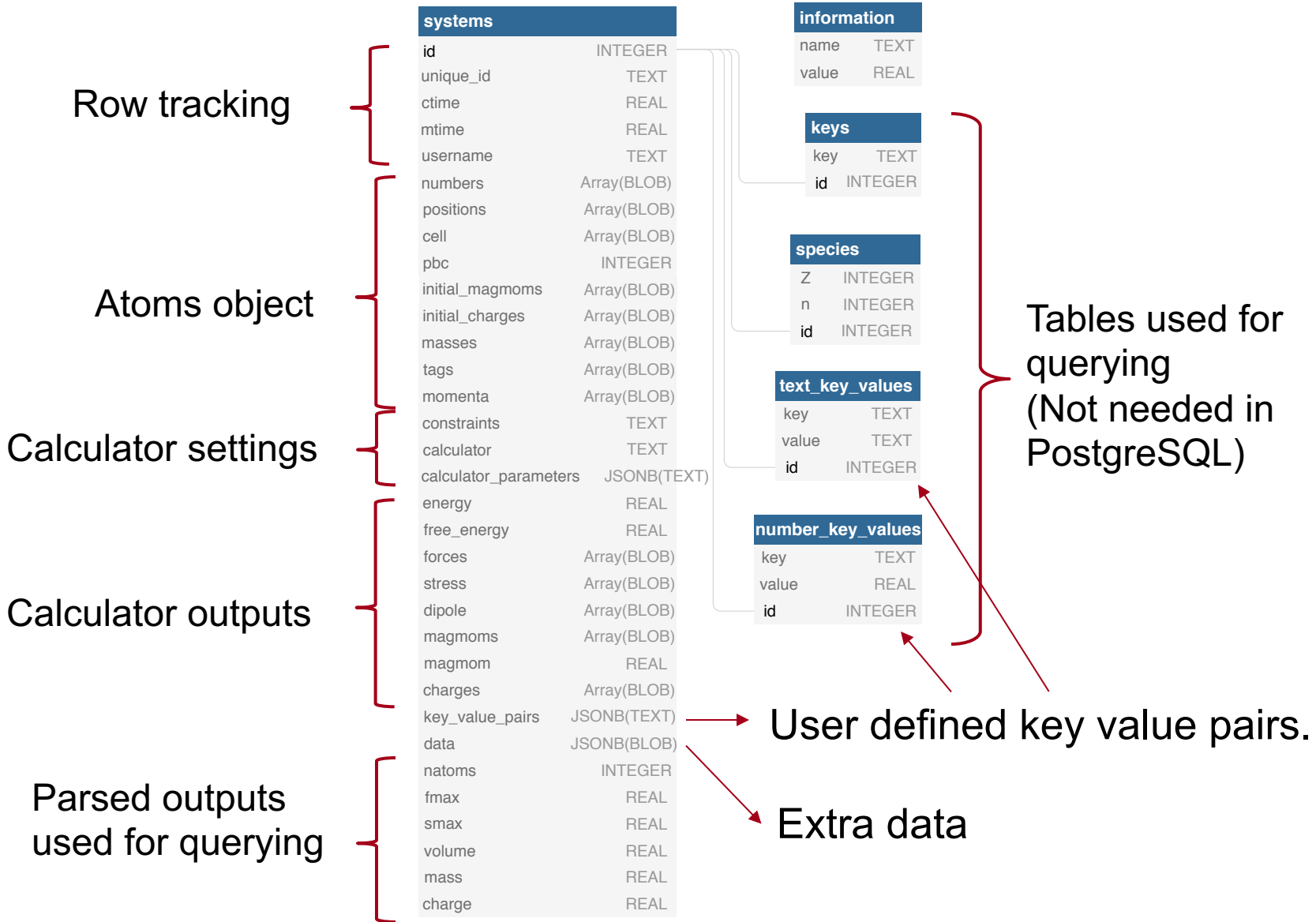
  - Local backends: 

  - Server side backends: 

- NoSQL (key value pair databases) 

  - No fixed database schema/structure -> high flexibility and scalability
  - PostgreSQL also has NoSQL-like features (JSONB data type)

Database structure (schema)



A simple use example

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```
#!/usr/bin/env python3

from ase.db import connect

db = connect('dbname.db'). # SQLite3 backend
db.write(atoms,
         key_value_pairs={'relaxed':1, adsorbate: 'C'}
         data={'vib': frequency_array})
# Select rows
for row in db.select('Cu', 'O>3', adsorbate='C'):
    print(row.id)
    print(row.energy)
    print(row.forces)
```

More examples at https://wiki.fysik.dtu.dk/ase/tutorials/db/db.html

Command line interface

View and sort calculations:

```
$ ase db AB2.db completed=1,relaxed=1 -s Ef -c
formula,p_name,energy,Ef,fmax,smax
formula|p_name          | energy|    Ef| fmax| smax
Ti2O4  |AB2_2_a_c_102  |-49.776|-8.476|0.008|0.038
Ti2O4  |AB2_2_d_j_84   |-49.766|-8.475|0.150|0.059
Ti4O8  |AB2_4_b_f_64   |-97.931|-8.341|0.013|0.034
Ti4O8  |AB2_4_j_lk_131|-97.738|-8.325|0.020|0.031
Ti4O8  |AB2_4_a_c_205  |-97.198|-8.280|0.007|0.032
Ti2O4  |AB2_2_a_b_224  |-48.386|-8.245|0.000|0.032
Ti4O8  |AB2_2_a_b_224  |-96.771|-8.245|0.002|0.033
```

Run local web-app:

```
$ ase db AB2.db -w
```

View structures in ASE gui:

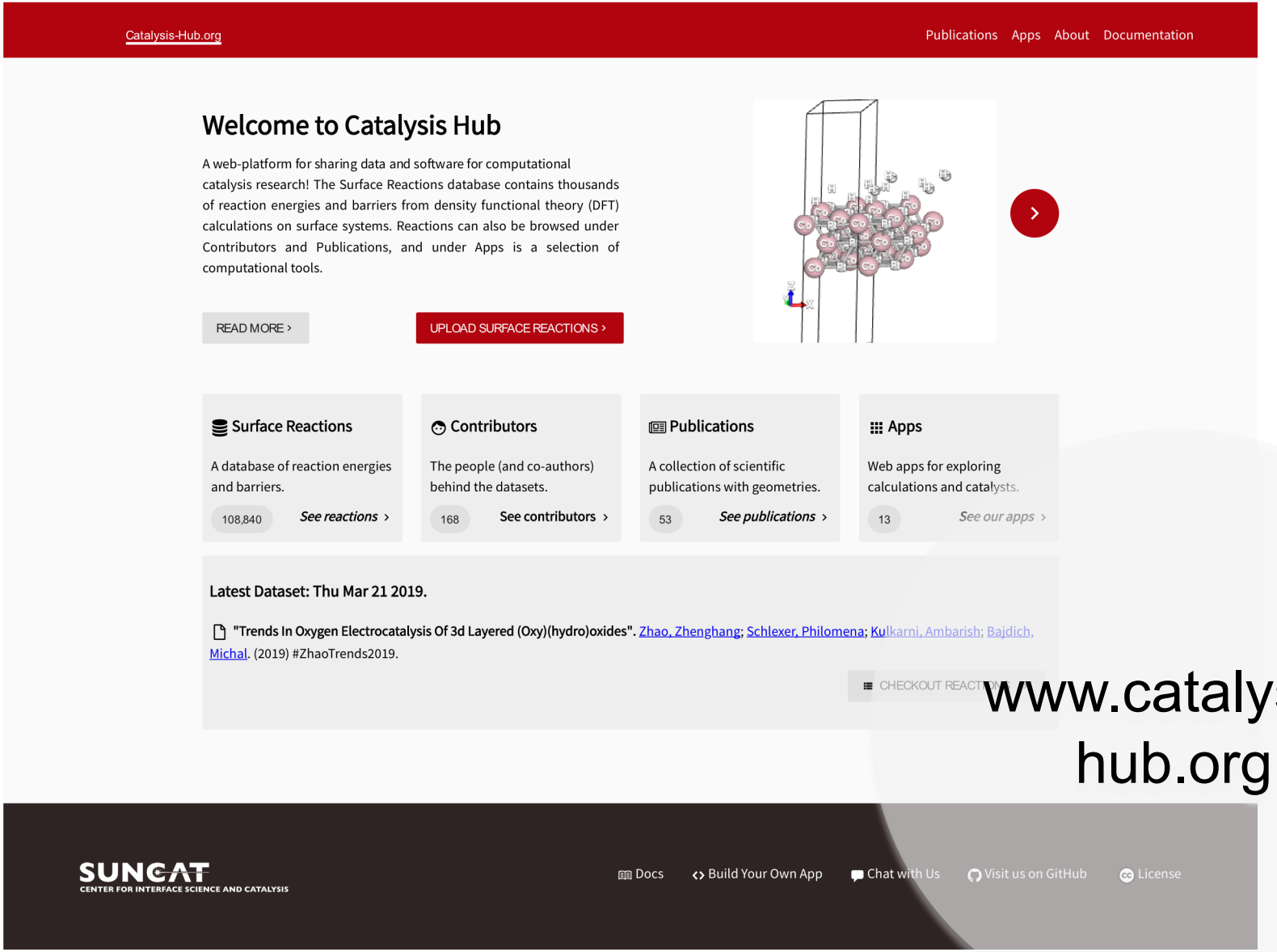
```
$ ase gui name.db@id=30
```

Server side databases using ASE db

- Computational Materials Repository: http://cmr.fysik.dtu.dk

- Katladb: https://nano.ku.dk/english/research/theoretical-electrocatalysis/katladb/

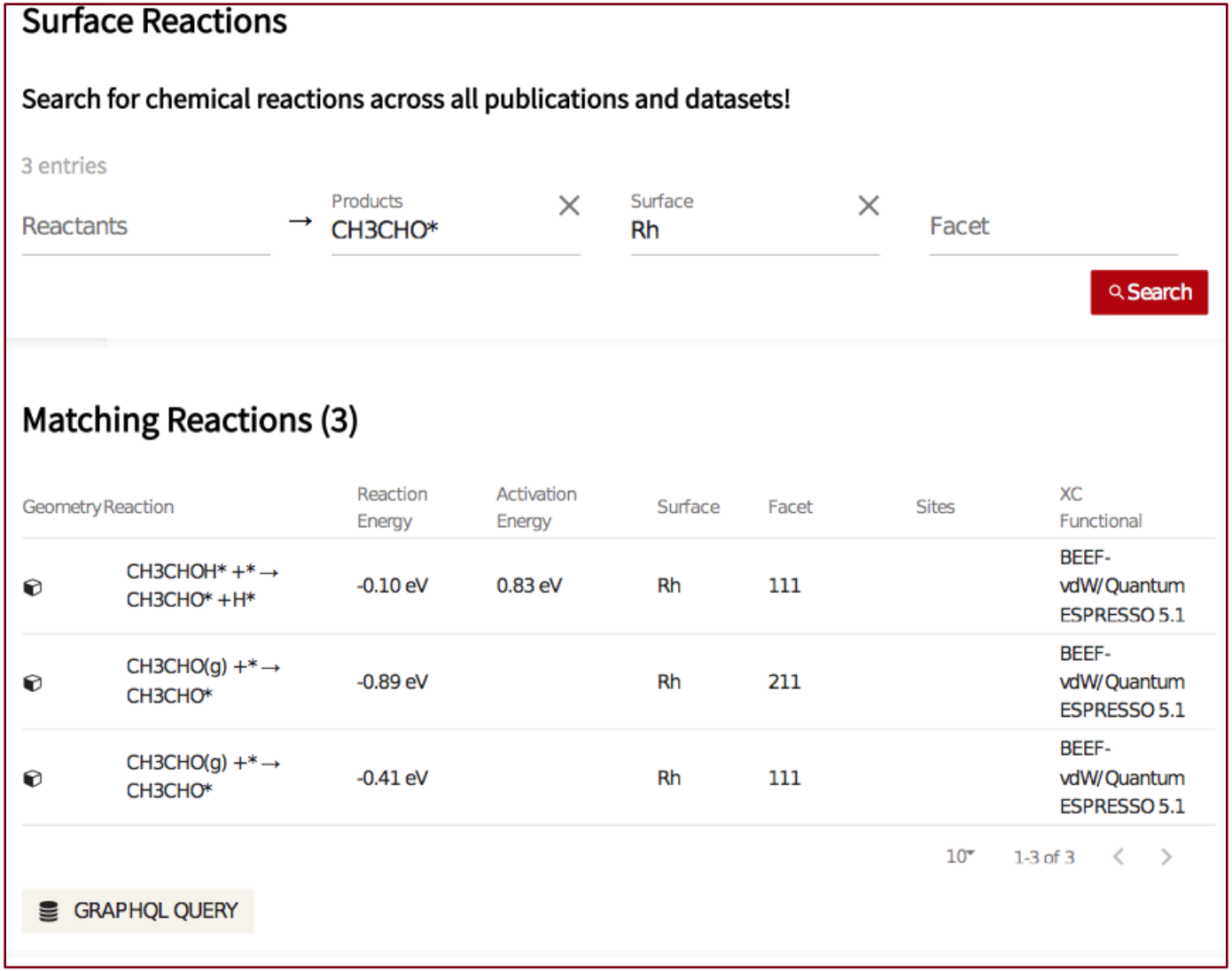
- Catalysis-hub: http://www.catalysis-hub.org



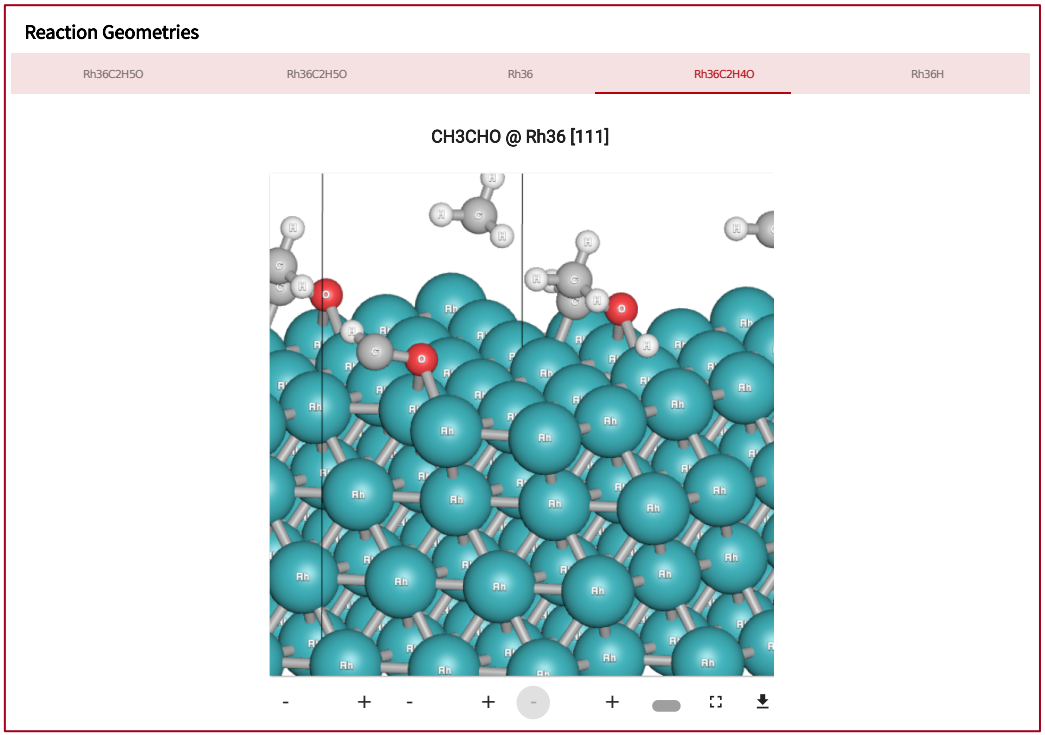
www.catalysis-hub.org

Winther, K.T. , Hoffmann, M. J., Mamun, O., Boes, J.R, Bajdich, M, Bligaard, T. Scientific Data (2019)

Surface Reactions database search



Visualize atomic structures in the browser

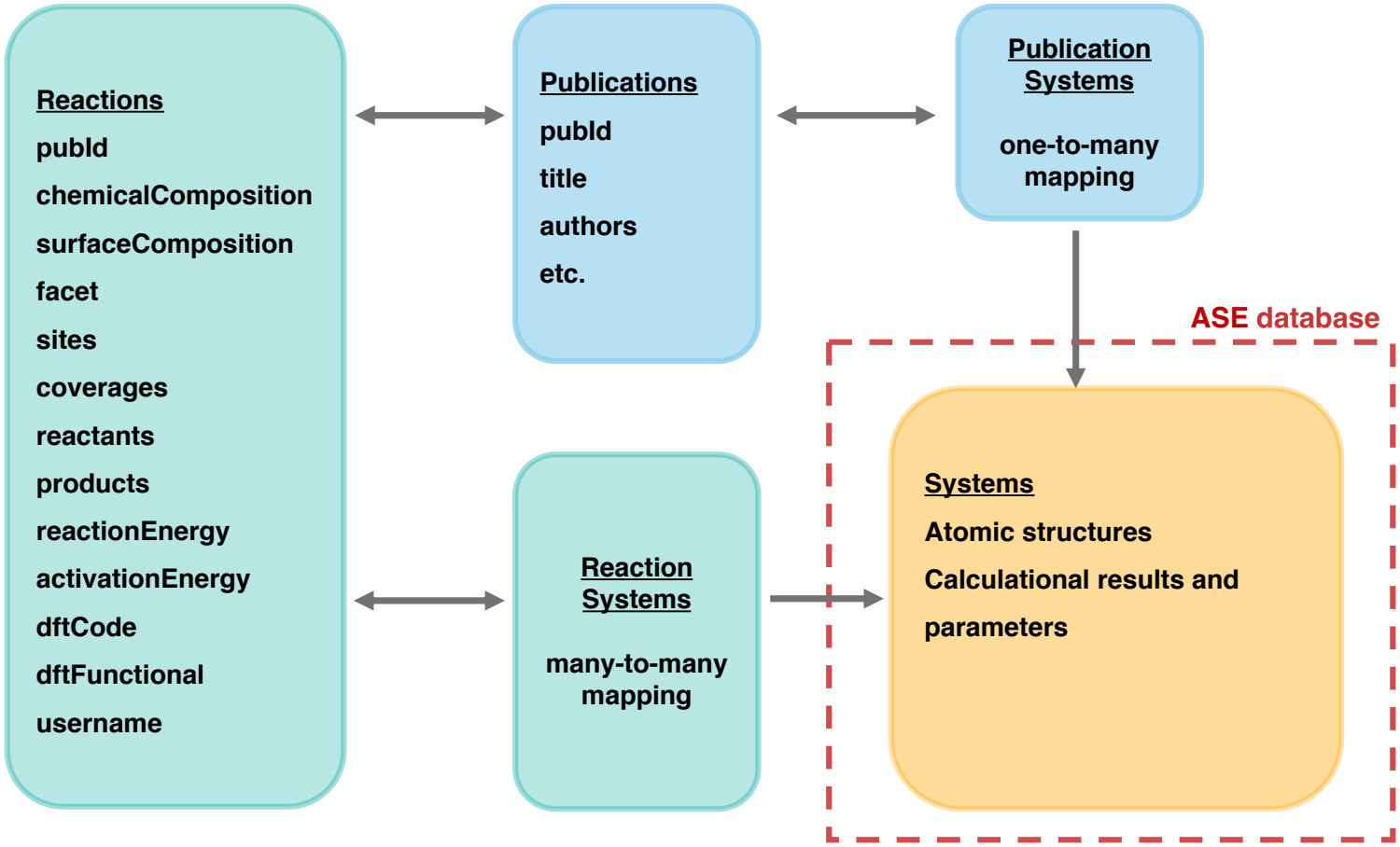


browse through all structures involved

View calculational details

- Formula: Rh36C2H4O
- DFT Total Energy: -115620.80 eV
- DFT Code: Quantum ESPRESSO 5.1
- DFT Functional: BEEF-vdW
- Publication: **"Selectivity Of Synthesis Gas Conversion To C2+ Oxygenates On Fcc (111) Transition-metal Surfaces"**. Schumann, Julia; Medford, Andrew J.; Yoo, Jong Suk; Zhao, Zhi-Jian; Bothra, Pallavi; Cao, Ang; Studt, Felix; Abild-Pedersen, Frank; Nørskov, Jens K.. *ACS Catalysis*. 4, 3447– 3453 (2018)
- Source DOI: 10.1021/acscatal.8b00201
- View all reactions in dataset
- Open GRAPHQL QUERY to view calculational details.

Catalysis-Hub data structure: extra tables

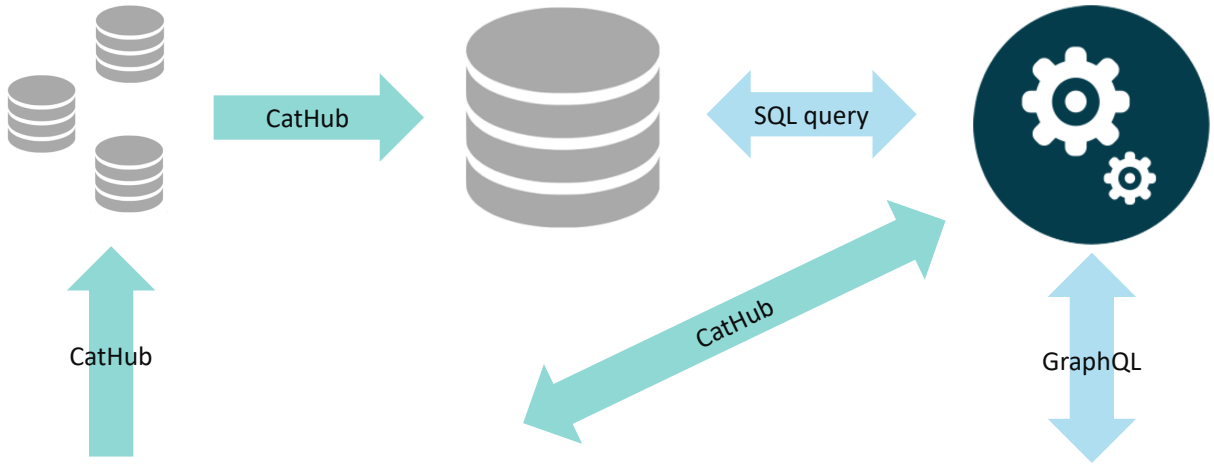


Catalysis-hub infrastructure

Data contributions
(SQLite3)

Database server
(PostgreSQL)

Web API (backend) at
https://api.catalysis-hub.org



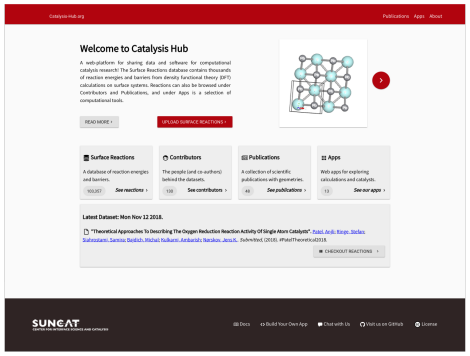

```
~$
~$ cathub reactions -q reactants=CO
Connecting to database at http://api.catalysis-hub.org/graphql

Executing query:

{reactions(first: 10, reactants: "CO") {
 totalCount
  edges {
    node {
      chemicalComposition
      Equation
      reactionEnergy
    }
  }
}}

Getting data from server...
```

Local workstation



Web page at
https://www.catalysis-hub.org

https://github.com/SUNCAT-Center

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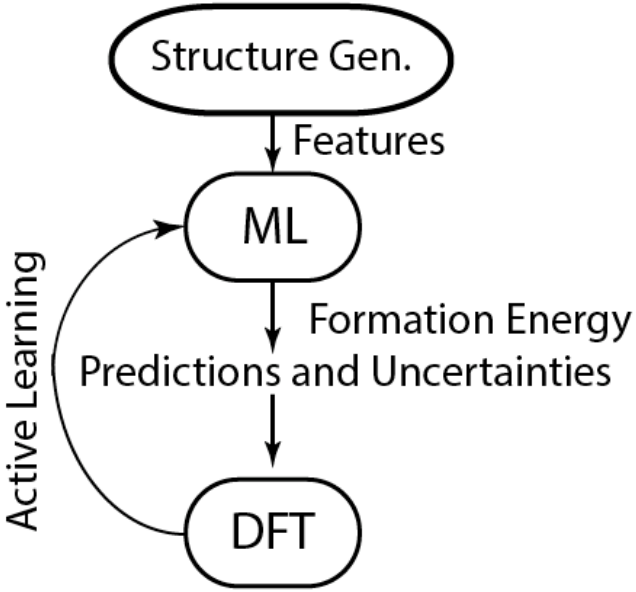
  - Machine learning workflows
- Suggested improvements and future plans.

Motivation: Beyond high-throughput computational screening

- We don’t want to calculate everything with DFT!
- Use machine learning to guide the search which will (hopefully) enable us to search a broader space of materials with less DFT calculations.
- In active learning the ML model is continuously retrained with new calculations

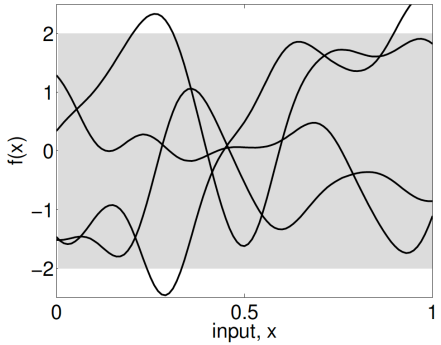


Machine learning for materials discovery

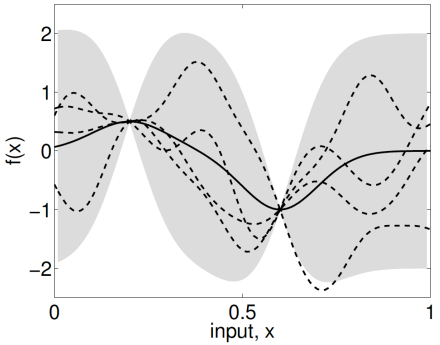
- Supervised regression with Gaussian Processes

$$y:\ \tilde{y} = f(X, \varphi)$$

target input features free parameters

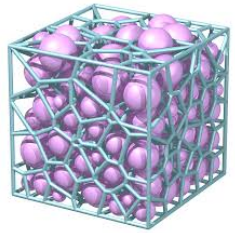


(a), prior



(b), posterior

- Fingerprint: Magpie voronoi tesselation[1]:

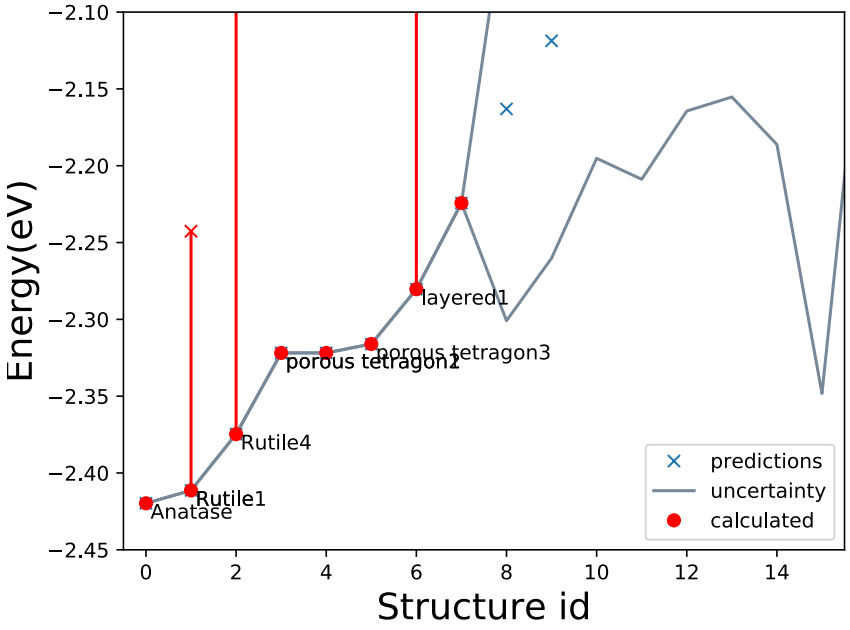


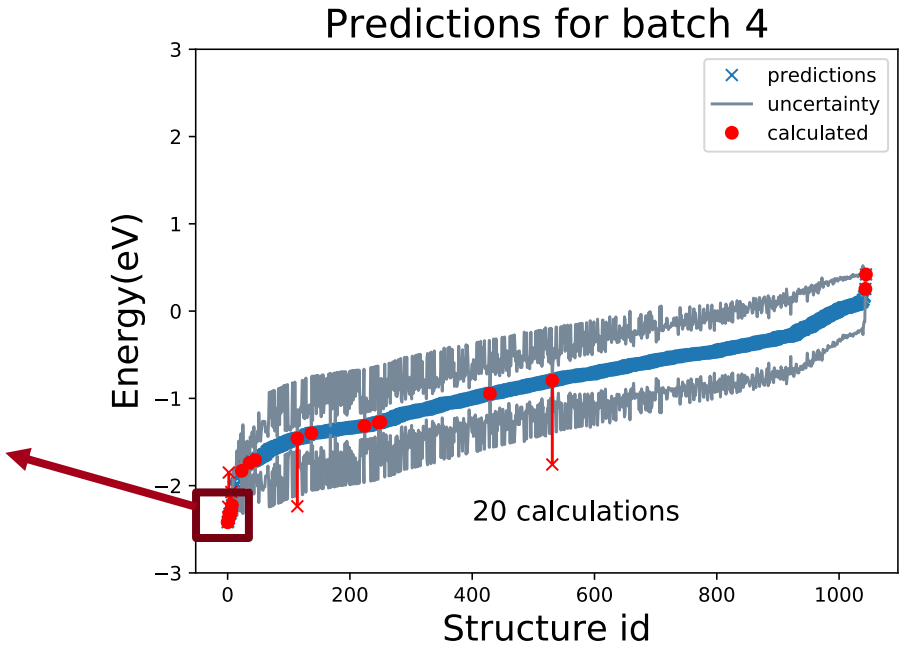
\+ 22 elemental properties (electronegativity, meting temperature, valence electrons, band gap, etc.) → 271 features for each structure

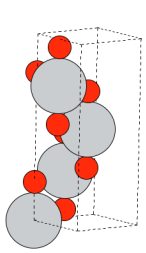
- Acquisition function: LCB = mean(Ef) – std(Ef)

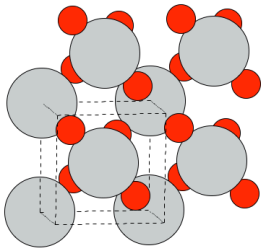
[1] L. Ward, C. Wolverton et al. PRB 96, 024104 (2017)
https://bitbucket.org/wolverton/magpie

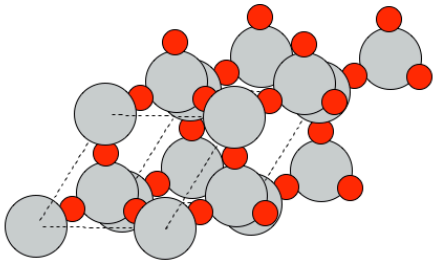
(Re)discovering stable polymorphs of TiO_2

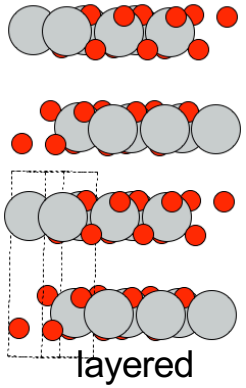





anatase


rutile


porous tetrahedral


layered

Automated acquisition, job submission and monitoring

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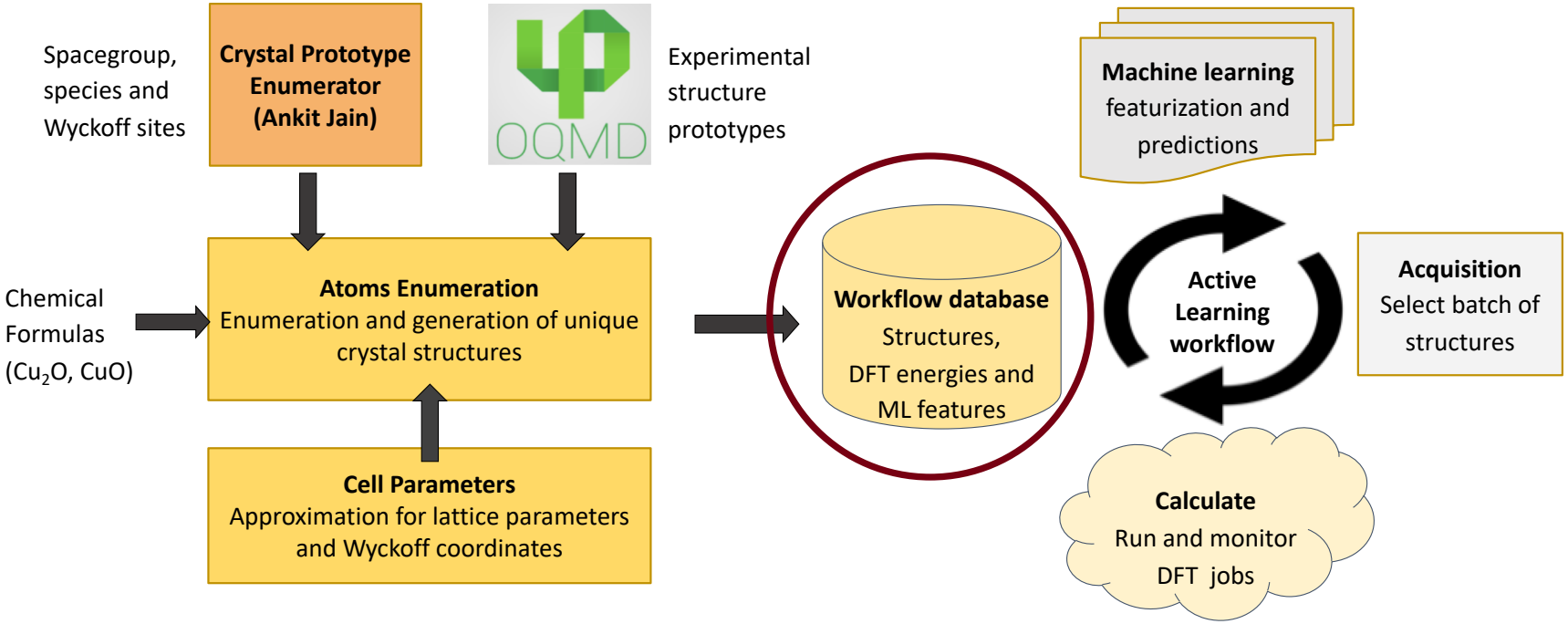
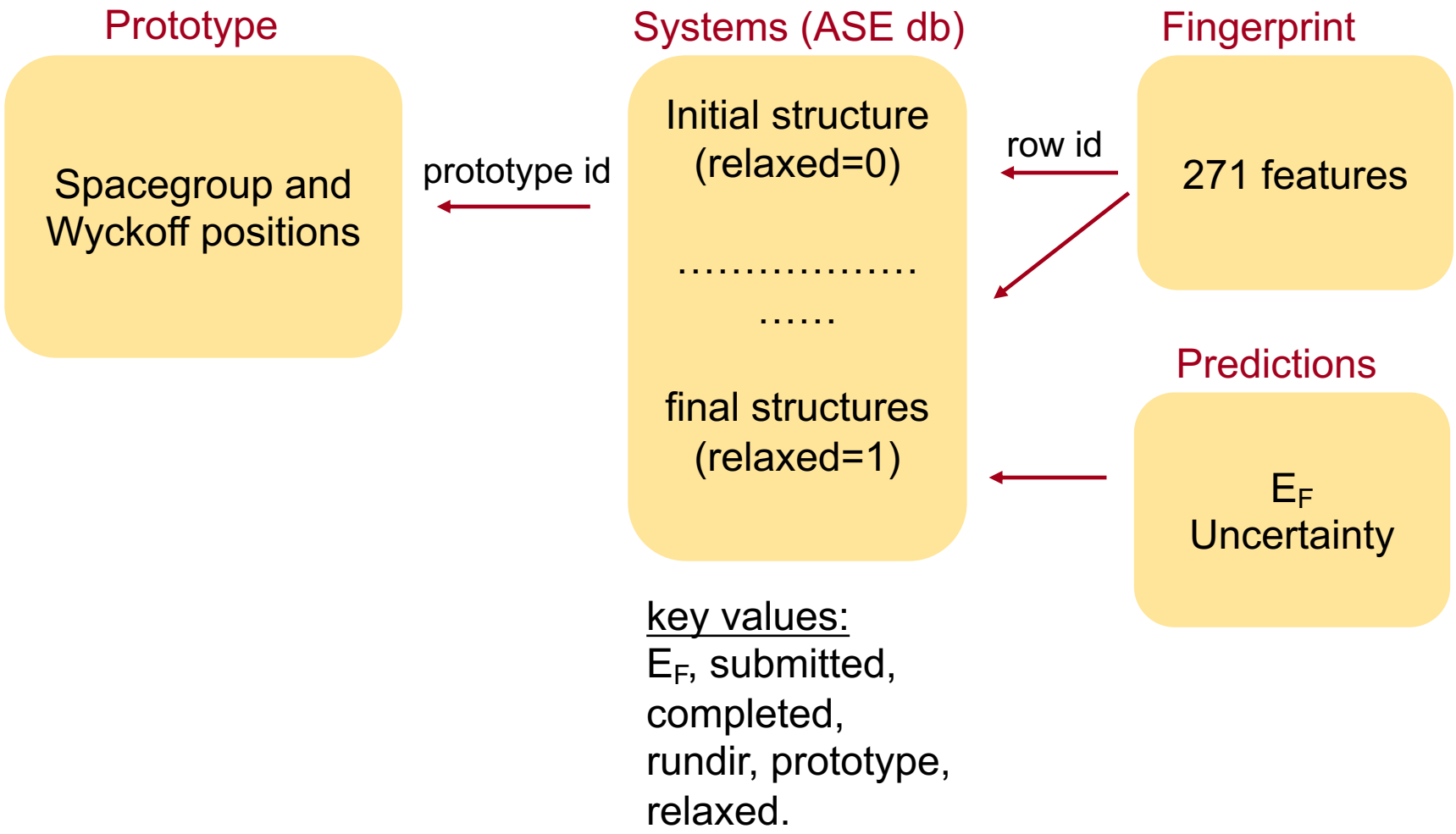


Workflow database structure



Possible improvements to the database

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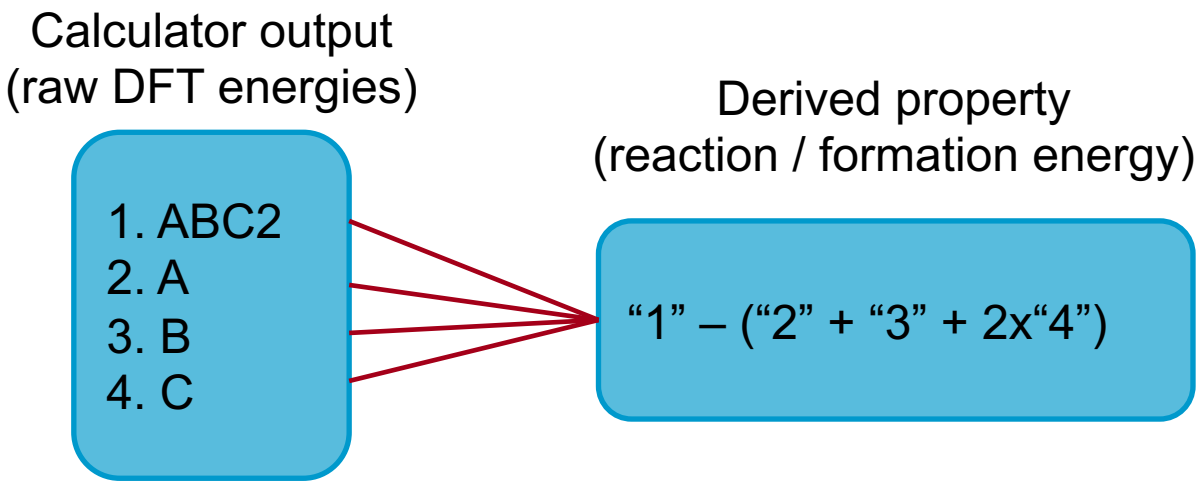
Handle connections between atoms-rows:

- Storing full relaxation pathway / NEB images:

- Connections between row to get derived properties.



Possible improvements continued …

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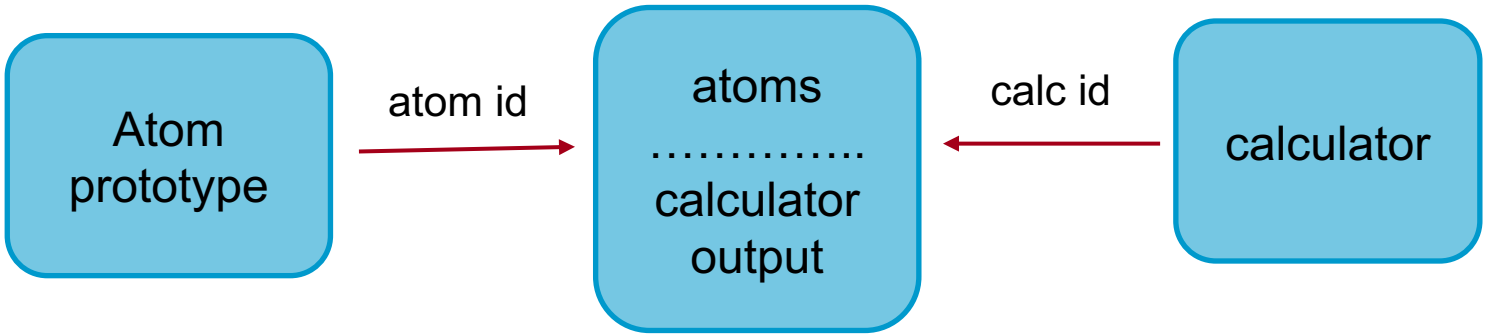
Calculator information for enhanced workflow and data sharing:

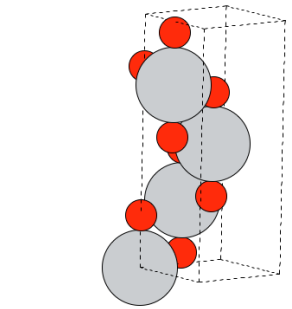
- Fix calculator ios + more tests (reading calculator and parameters from raw input/output files)
- Calculator version + setups/potentials!
- Storing detailed calculator output such as eigenvalues?
- Efficient grouping of entries with same calculator settings in separate 'Calculator' table?



Other possible contributions

- Extension to the Spacegroup module to include Wyckoff positions:

```
crystal(symbols=[‘Ti’, ‘O’],
        wyckoffs=[’a’, ‘e’],
        spacegroup=141,
        cellpar={‘a’: 3.78, ‘b’: 3.78, ‘c’: 9.51,
                 ’alpha’: 90, ‘beta’: 90,
                 ‘gamma’: 90,
                 ‘e1z’: 0.21})
```



anatase

- Structural fingerprints for machine learning?

Ackowledgements

DTU

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Osman Mamun

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Raul Flores

Ankit Jain

Meng Zhao

Chris Paolucci

SUNCAT postdocs

TRI Materials:

Jens Hummelshøj

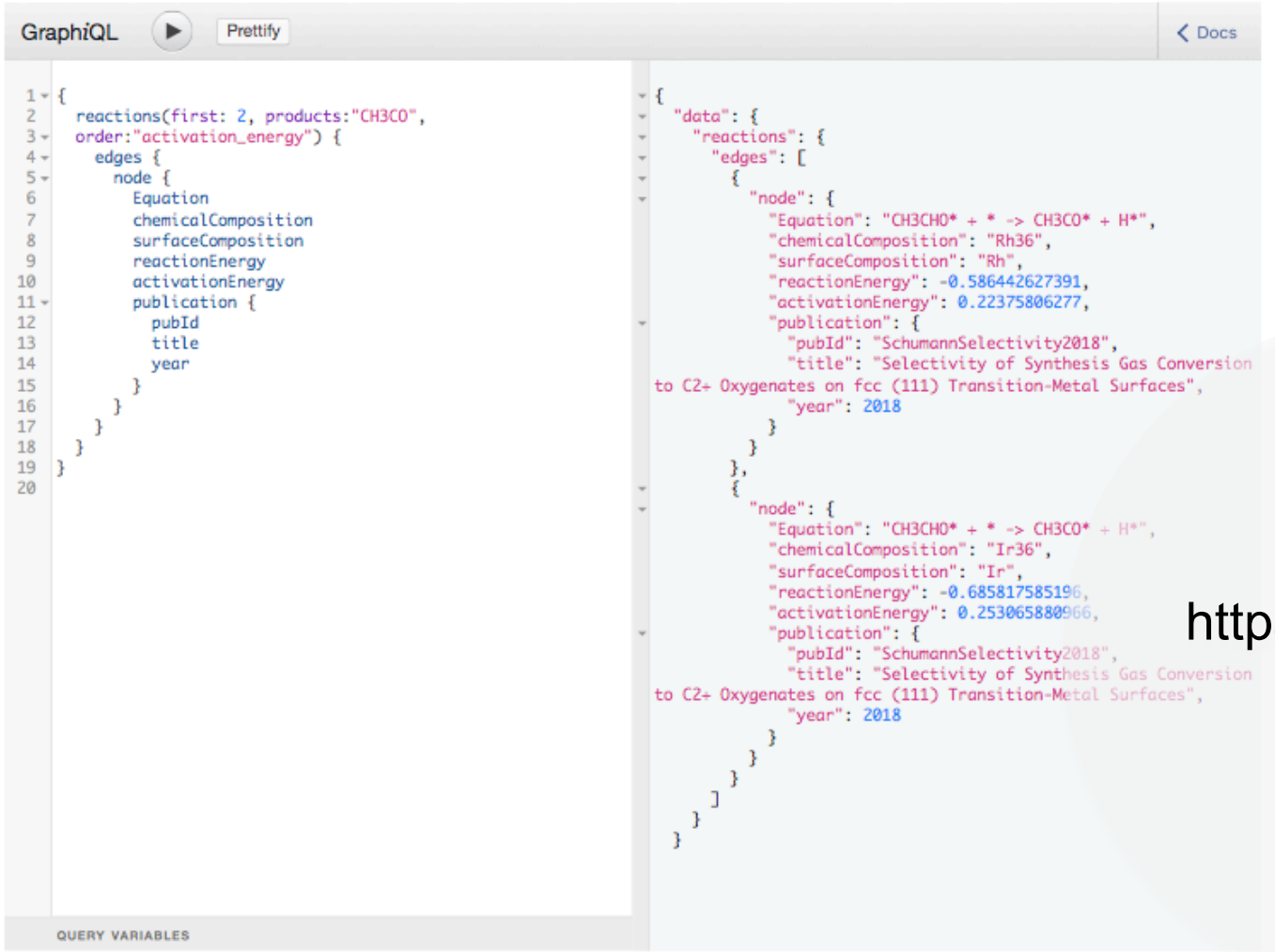
Joseph Montoya

Murat Aykol

Thank you for your attention

… and please share your data!

Direct access to data in web API



https://api.catalysis-hub.org

Materials databases