Our software ecosystem for data-driven research

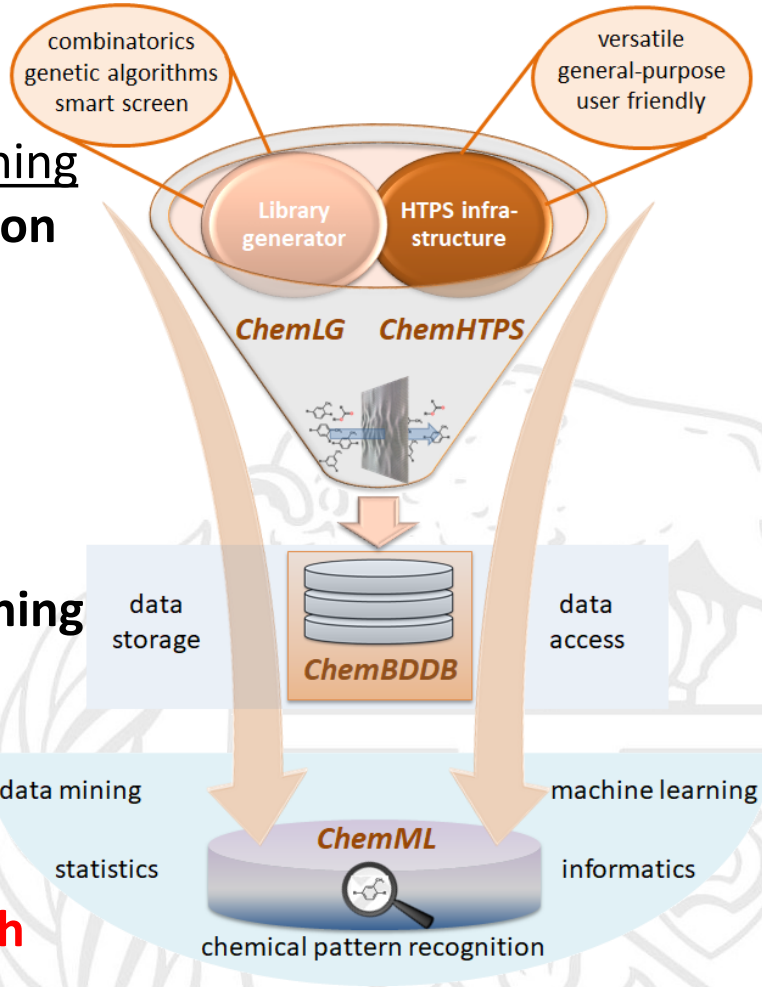
University at Buffalo
The State University of New York

ChemLG: a smart library generator for the **definition and enumeration** of chemical and materials spaces

ChemHTPS: an automated high-throughput screening platform for chemical and materials **data generation**

ChemBDDB: a big data database template for chemical and materials **data storage**

ChemML: a machine learning and informatics program suite for chemical and materials **data mining**



- **make state-of-the-art data science a viable proposition in chemical and materials research**

Mol Sim 44 (**2018**), 921

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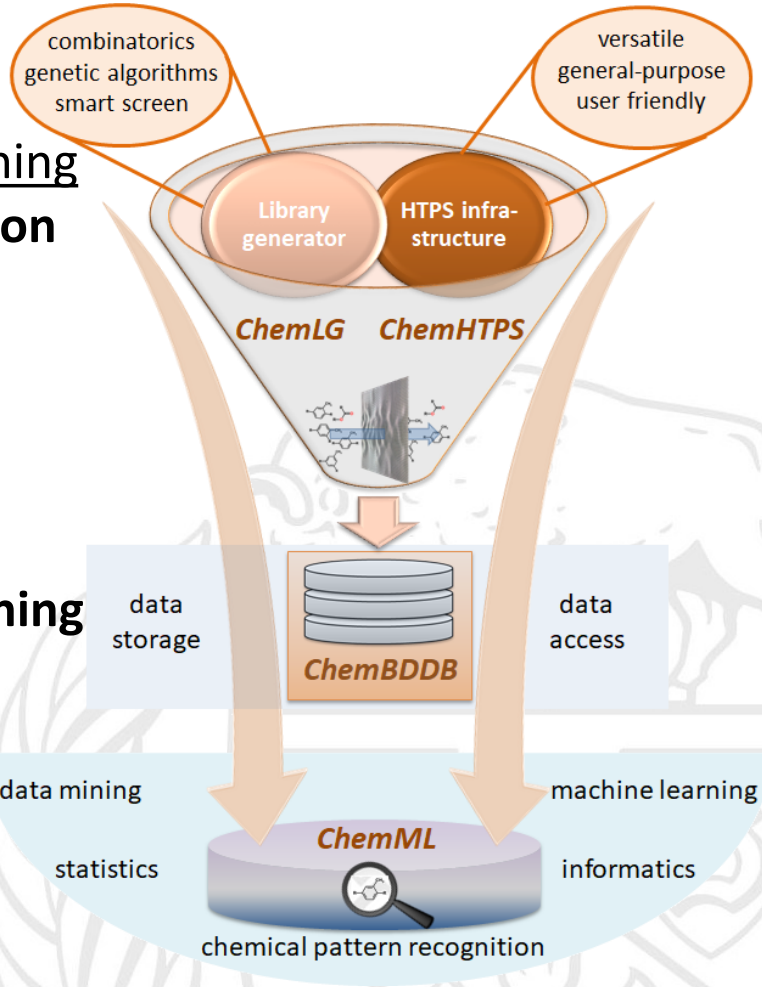

- as **general-purpose, comprehensive, user-friendly,** and **automated** as possible

Mol Sim 44 (**2018**), 921

ChemML: ML for chemical, materials data

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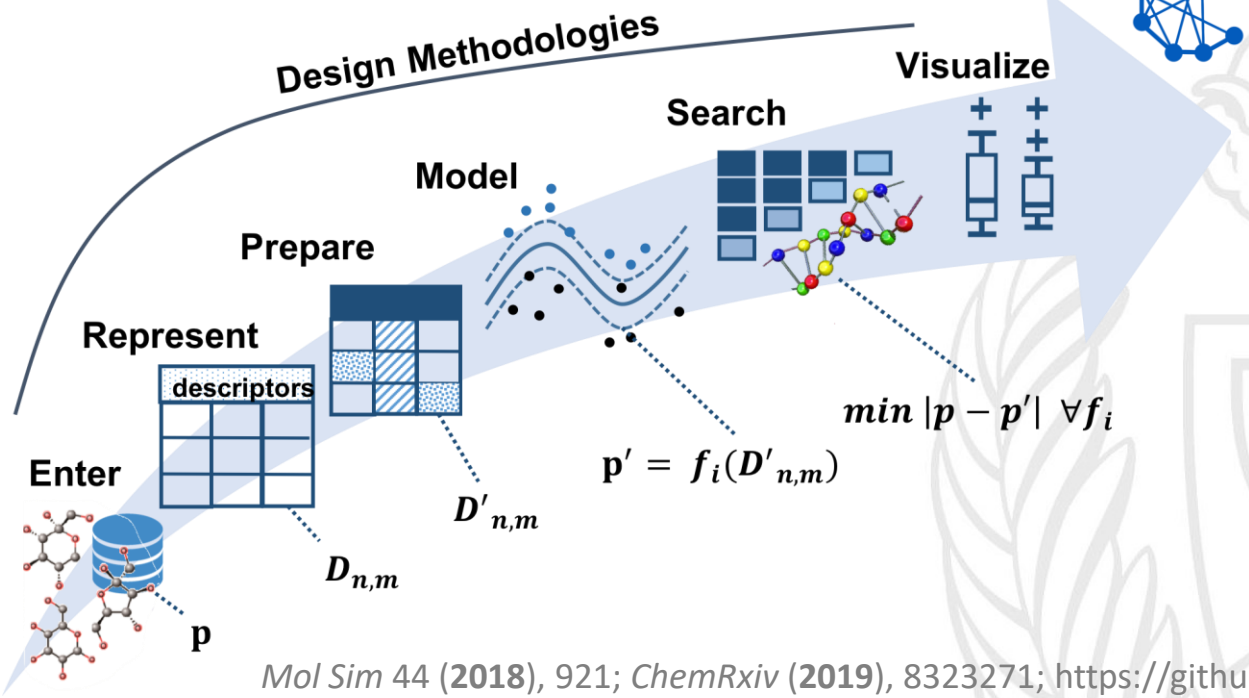
- goals: facilitate ML following example of QC program packages
  - staging and integration of tools (bridging chemical/materials, data domains)
  - abstraction of complex workflows
  - built-in expert knowledge, safeguards
  - development platform for methodological innovation
  - intuitive user experience



Mol Sim 44 (**2018**), 921; *ChemRxiv* (**2019**), 8323271; https://github.com/hachmannlab/chemml

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Quantum Chemistry Package

- specify geometry, charge, spin
  - ➢ define problem of interest (i.e., Hamiltonian)
- specify method (e.g., B3LYP/6-31G*)
- specify target property (e.g., dipole)
- specify algorithms, parameters (e.g., thresholds, cutoffs)

➢ code then executes job by calling appropriate series of modules and passing data

ChemML

- specify data set and its nature
  - ➢ define problem of interest
- specify method (e.g., TBFS-RR) or opt
- specify target property implied by data
- specify algorithms, parameters or opt (e.g., thresholds, cutoffs)

➢ code then executes job by calling appropriate series of modules and passing data (challenge to establish abstracted, generalized workflows)

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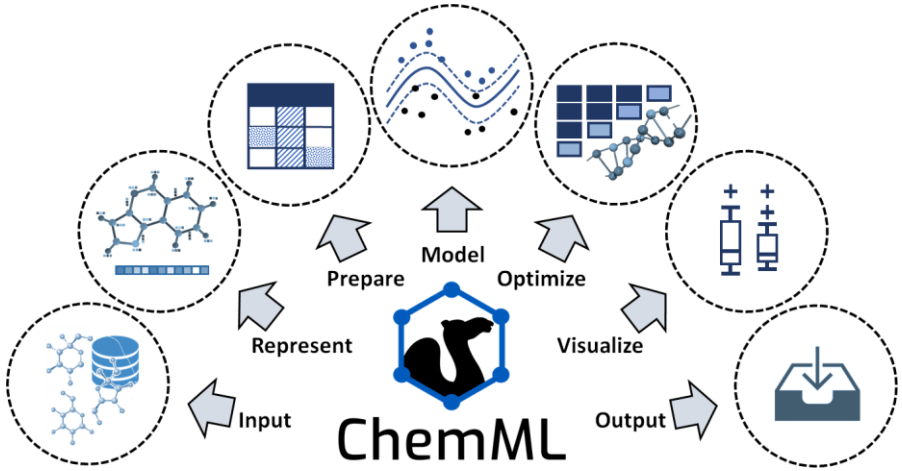

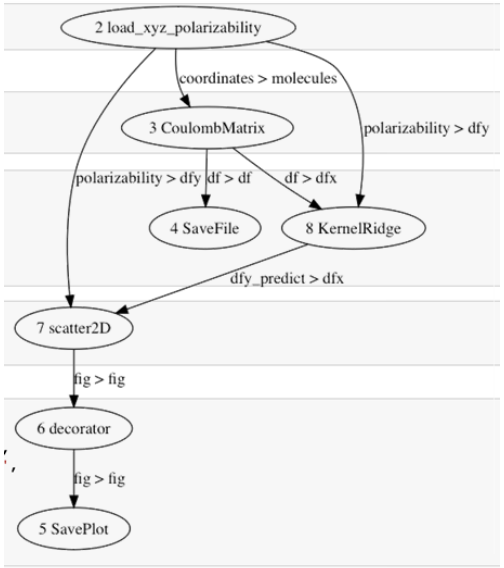

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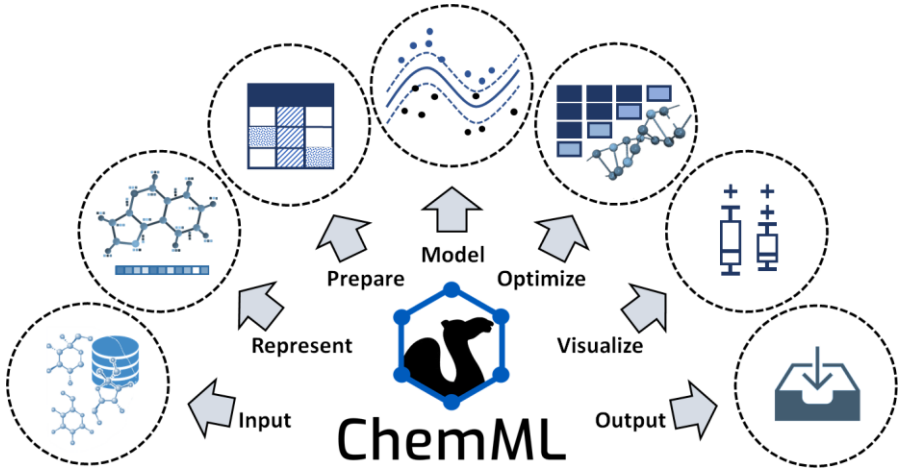


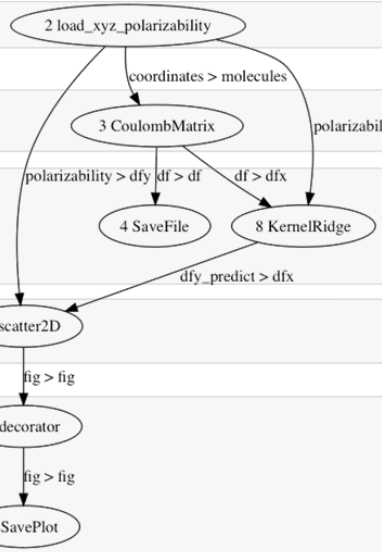

```
from chemml.datasets import load_xyz_polarizability
coordinates, polarizability = load_xyz_polarizability()
```

```
from chemml.chem import CoulombMatrix
model = CoulombMatrix()
df = model.represent(coordinates)
```

```
import pandas as pd
from sklearn.kernel_ridge import KernelRidge
clf = KernelRidge(kernel='rbf', alpha=0.1)
clf.fit(df,polarizability)
dfy_predict = clf.predict(df)
dfy_predict = pd.DataFrame(dfy_predict)
```

```
from chemml.visualization import scatter2D
sc = scatter2D(marker = 'o')
fig = sc.plot(polarizability, dfy_predict,0,0)
```

```
from chemml.visualization import decorator
dec = decorator(title = 'training performance',
                xlabel = 'predicted polarizability (Bohr^3)',
                ylabel = 'calculated polarizability (Bohr^3)',
                grid = True,
                grid_color = 'green'
                )
dec.matplotlib_font(size = 12)
fig = dec.fit(fig)
```



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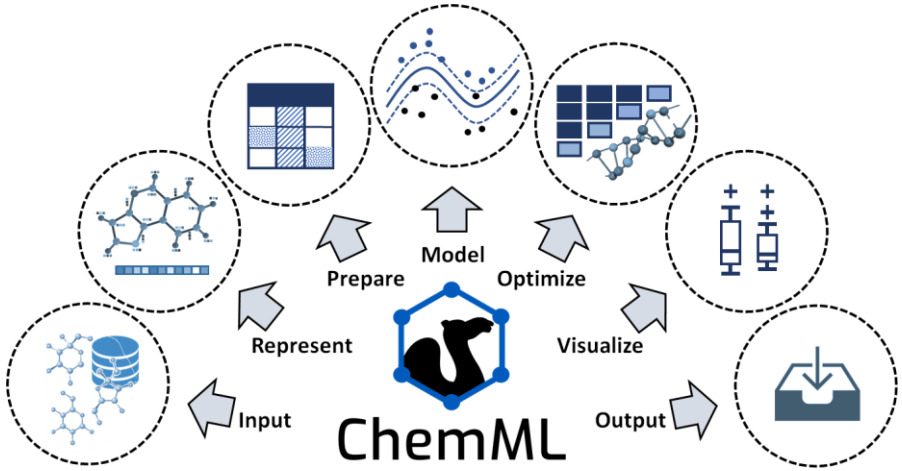


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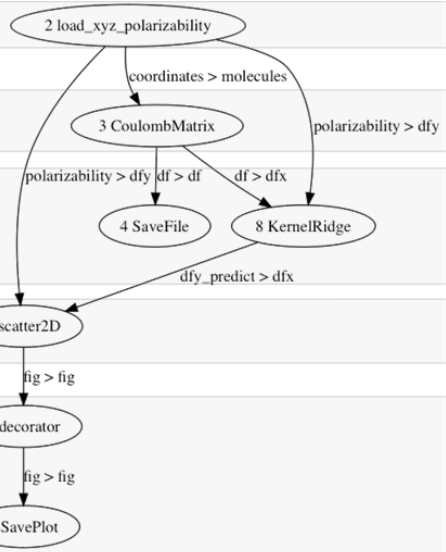


```
## (Enter,datasets)
    << host = cheml
    << function = load_xyz_polarizability
    >> coordinates 0
    >> polarizability 4
    >> polarizability 5

## (Represent,molecular descriptors)
    << host = cheml
    << function = CoulombMatrix
    >> 0 molecules
    >> df 1
    >> df 6

## (Store,file)
    << host = cheml
    << function = SaveFile
    << filename = CM_features
    >> 1 df

## (Store,figure)
    << host = cheml
    << function = SavePlot
    << kwargs = {'normed':True, 'bbox_inches':'tight'}
    << output_directory = plots
    << filename = performance
    >> 2 fig

## (Visualize,artist)
    << host = cheml
    << function = decorator
    << title = training performance
    << grid_color = g
    << xlabel = predicted polarizability (Bohr^3)
    << ylabel = calculated polarizability (Bohr^3)
    << grid = True
    << size = 12
    >> fig 2
    >> 3 fig
```

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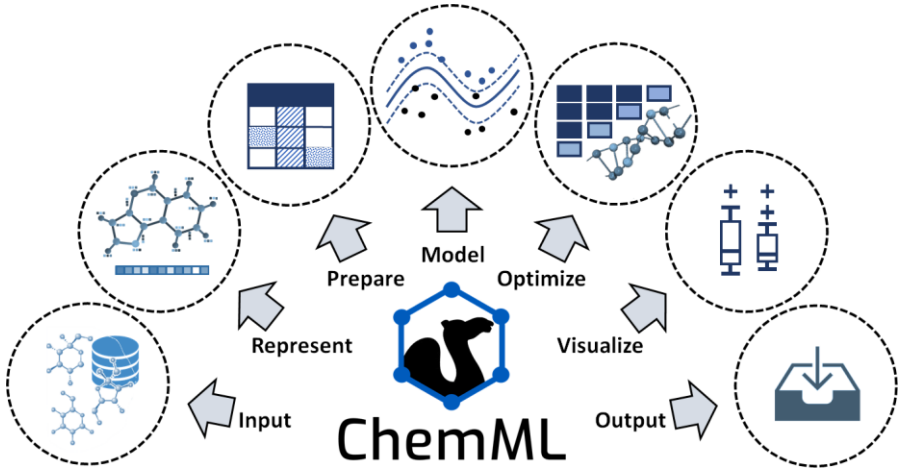

MaDE@UB

Open Chemistry

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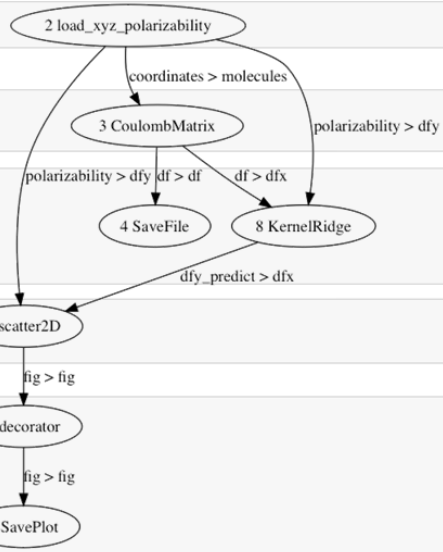


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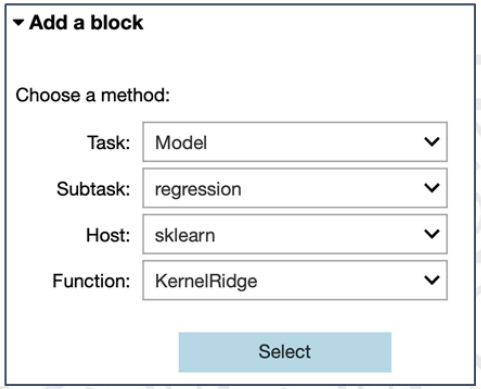

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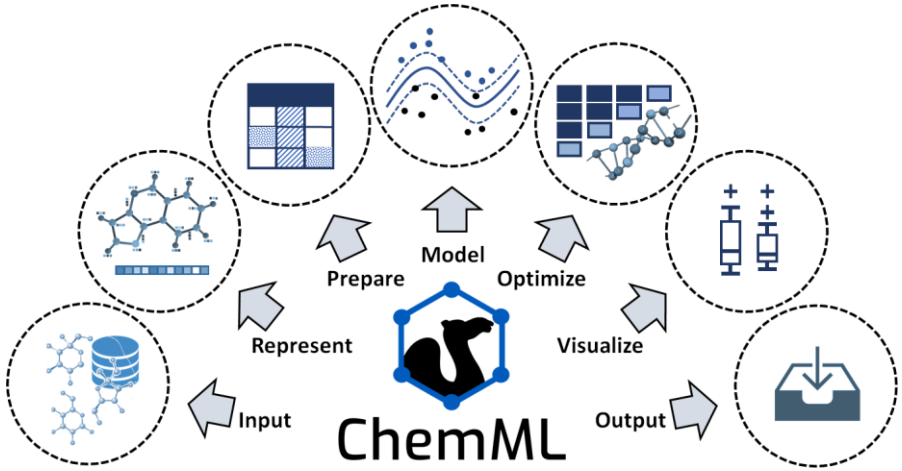

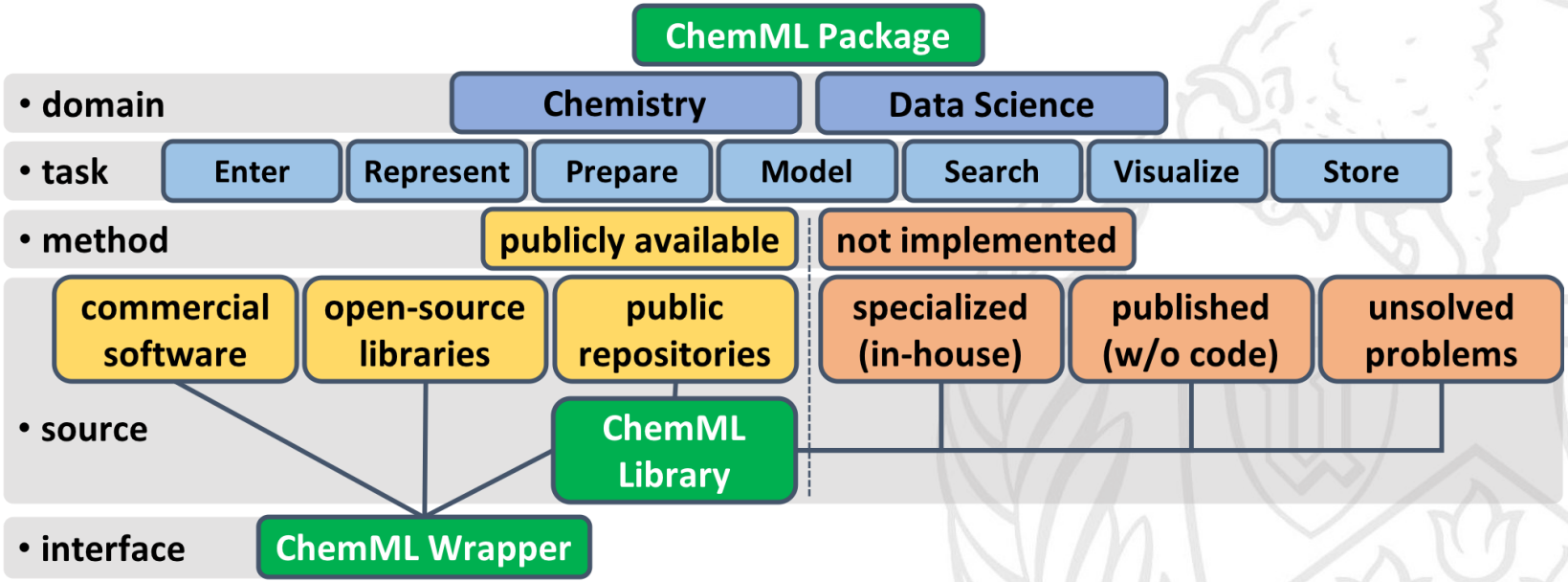

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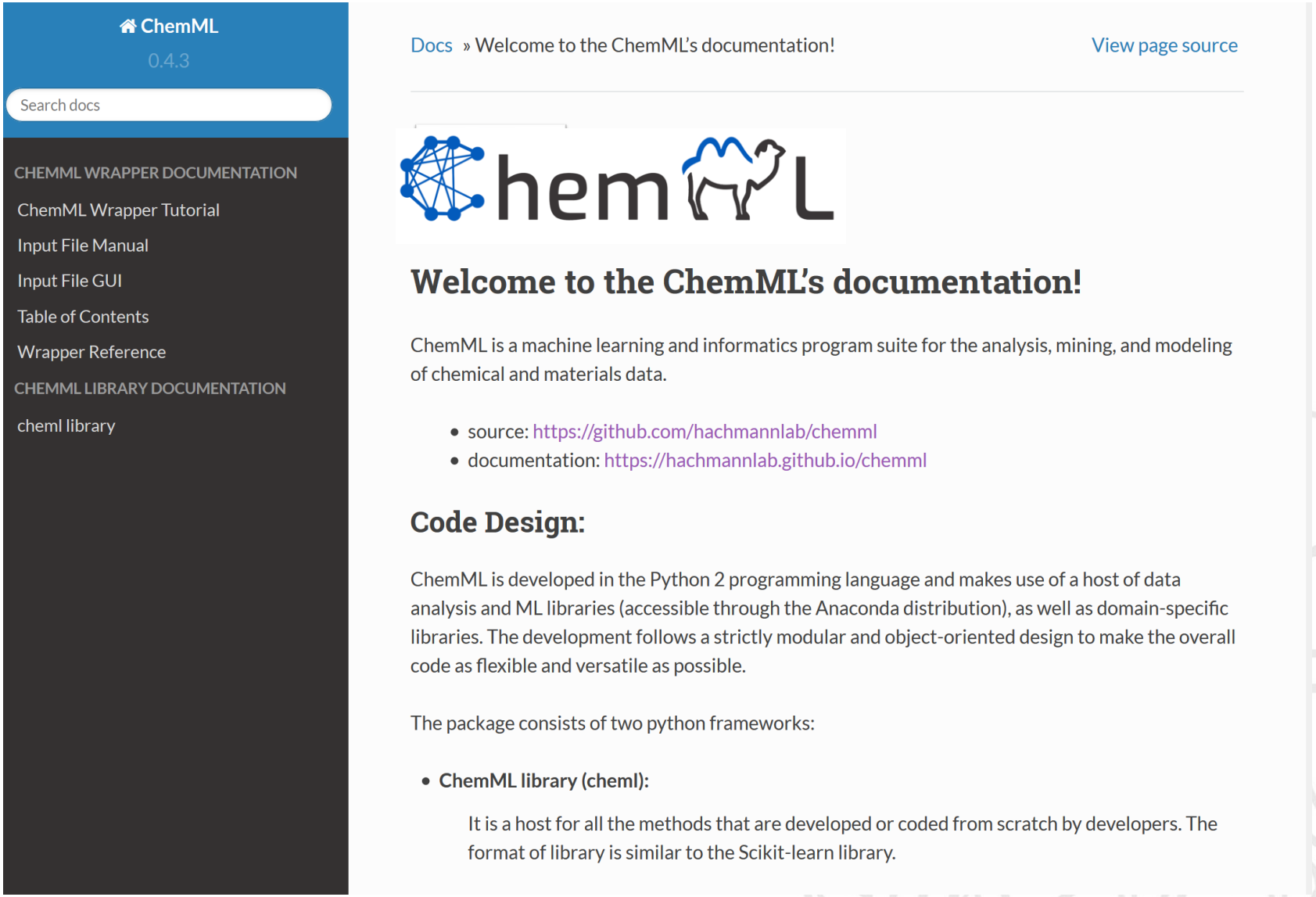

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