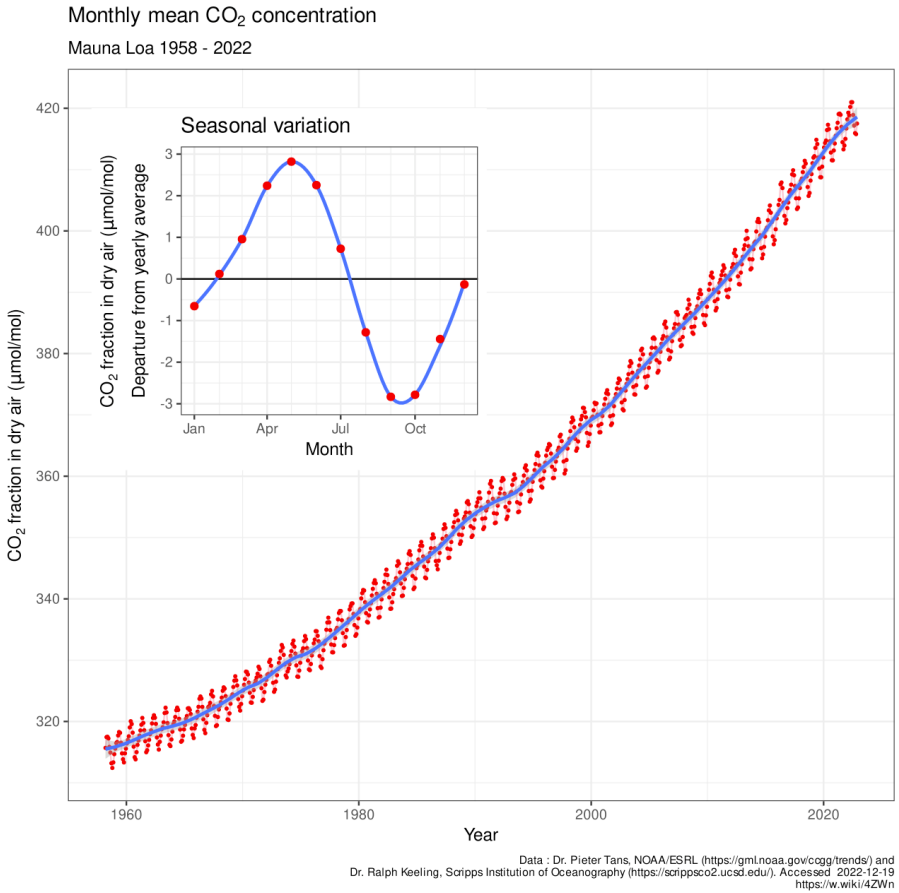
Adsorption using AiiDA Lab

CH-315

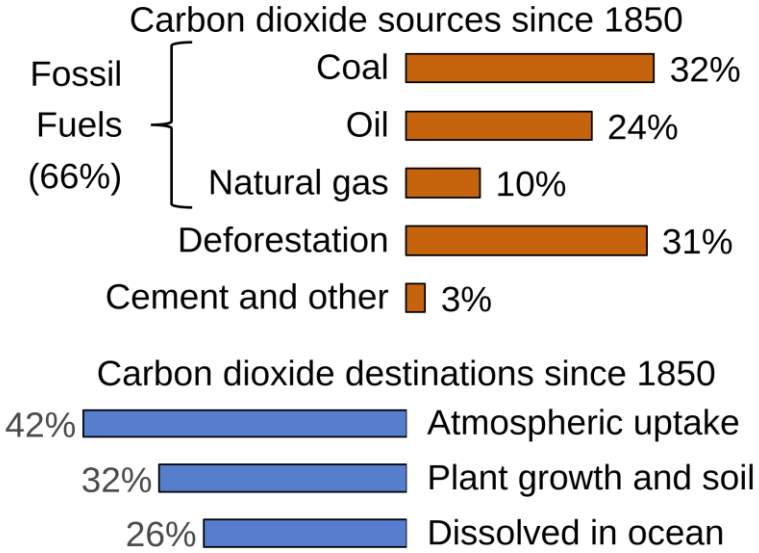
Assignment 2

26.9.2025

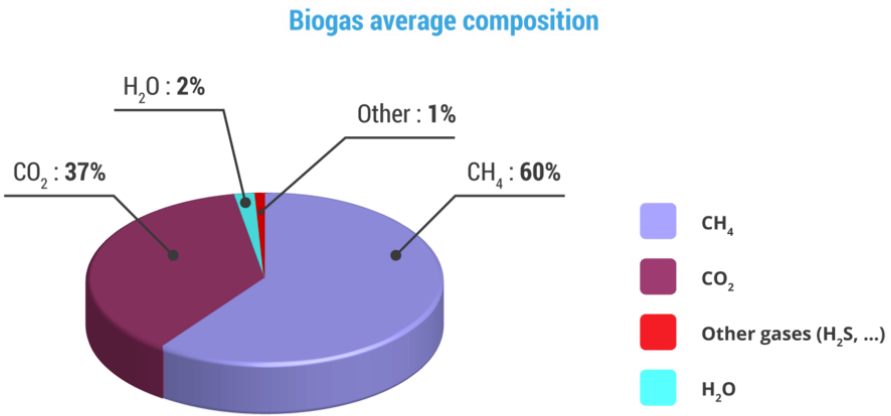
CO_2 concentration



Data : Dr. Pieter Tans, NOAA/ESRL (https://gml.noaa.gov/ccgg/trends/) and
Dr. Ralph Keeling, Scripps Institution of Oceanography (https://scrippsco2.ucsd.edu/). Accessed 2022-12-19
https://w.wiki/4ZWn



Typical composition of biogas



Challenges:

- CO_2/CH_4 separation
- Methane storage

In hand_on.pdf, you need to evaluate IRMOF-1 for these two applications

Flue gas

Flue gas conditions	NGCC
Flowrate (tonne/hr)	2268
Temperature (°C)	100
Composition (mol %)	-
CO_2	4.97
N_2	74.28
O_2	9.73
H_2O	11.02

Challenges:
- CO_2/N_2 separation
- CO_2/H_2O separation

In project.pdf, you need to screen 8 structures for CO_2/N_2 separation

Key Performance Indicator (KPI)

KPI: standard to evaluate MOFs

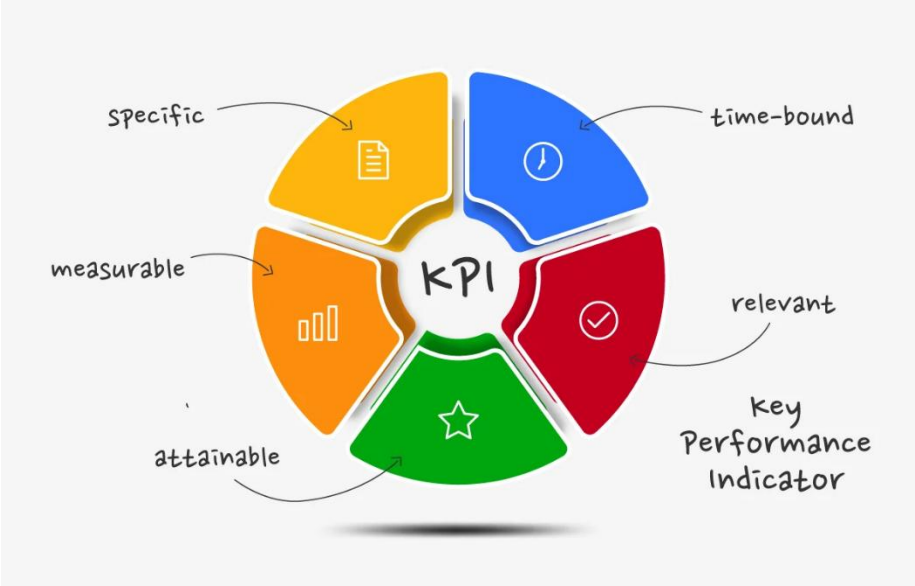
Important and direct property:

- Working Capacity
- Selectivity

Indirect property:

-Henry coefficient

-Pore volume



Working Capacity: important for storage and separation

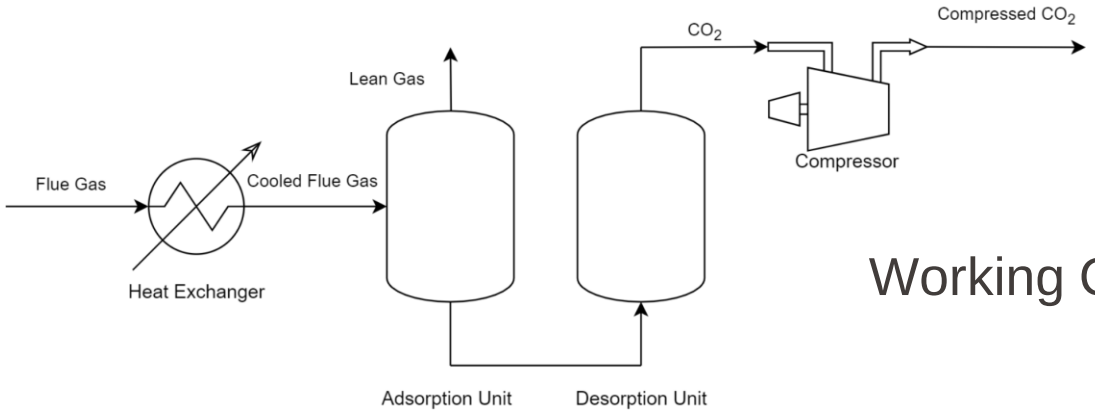
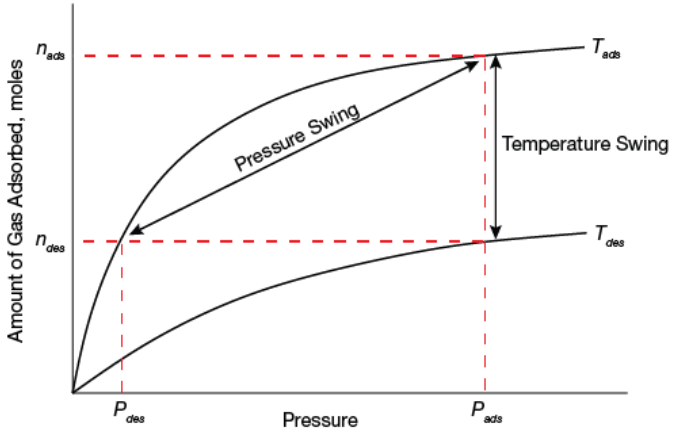


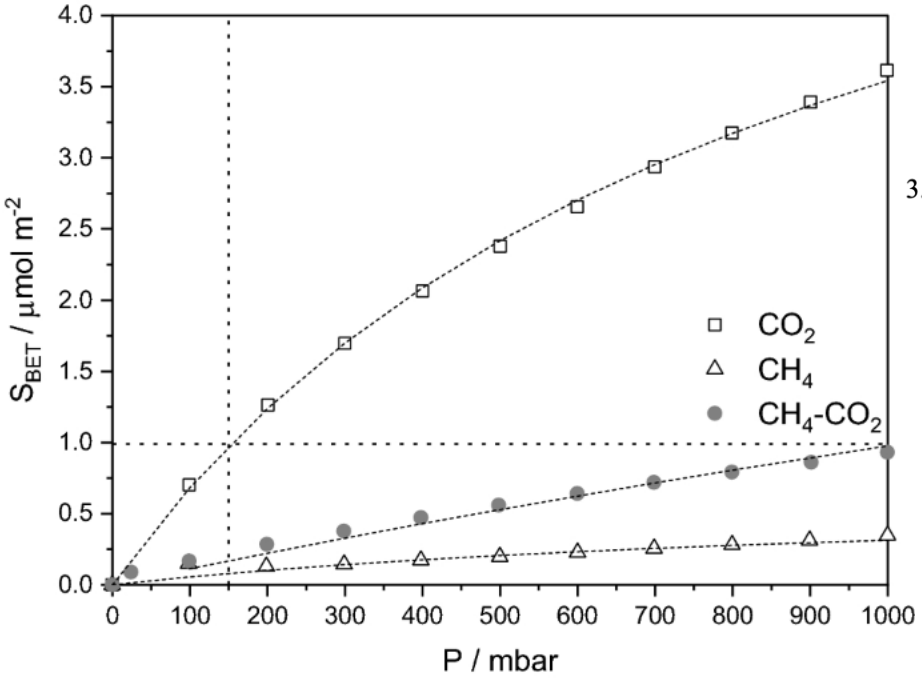
Figure 1: Flow diagram of the PSA/VSA process

Industry Process

Working Capacity obtained from Isotherm



Selectivity: important for storage



3. The ideal selectivity gives an indication on the competitiveness of adsorption between the different components of a gas mixture:

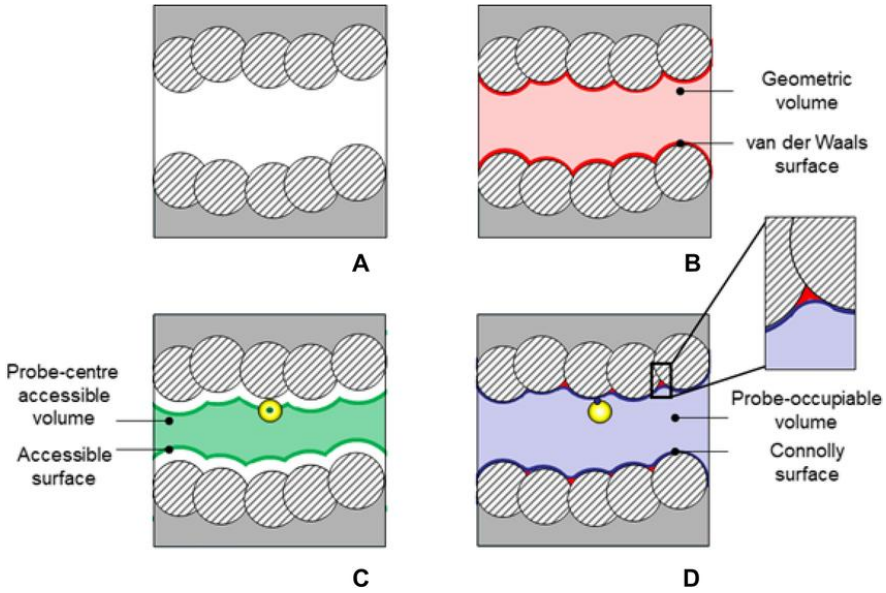
$$S_{CO_2/N_2} = \frac{q_{CO_2}}{q_{N_2}} \frac{y_{N_2}}{y_{CO_2}}$$

Where q is the binary loading, obtained from IAST calculations, at the adsorption conditions in mmol.g^{-1}, and y is the molar fraction of the component in the flue gas.

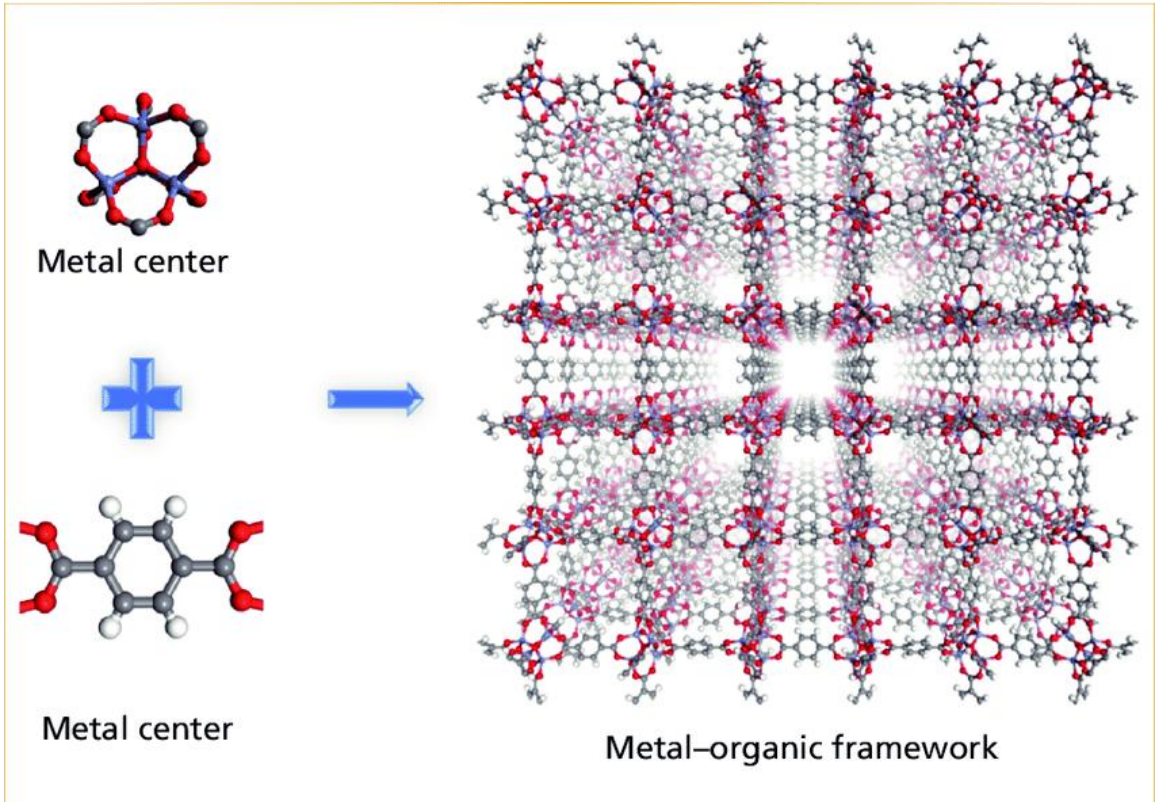
Indirect properties: Pore Volume and Henry Coefficient

-Henry coefficient

-Pore volume:
  -Done by zeo++
  -Insert a ball to detect (probe radius = 1.525)

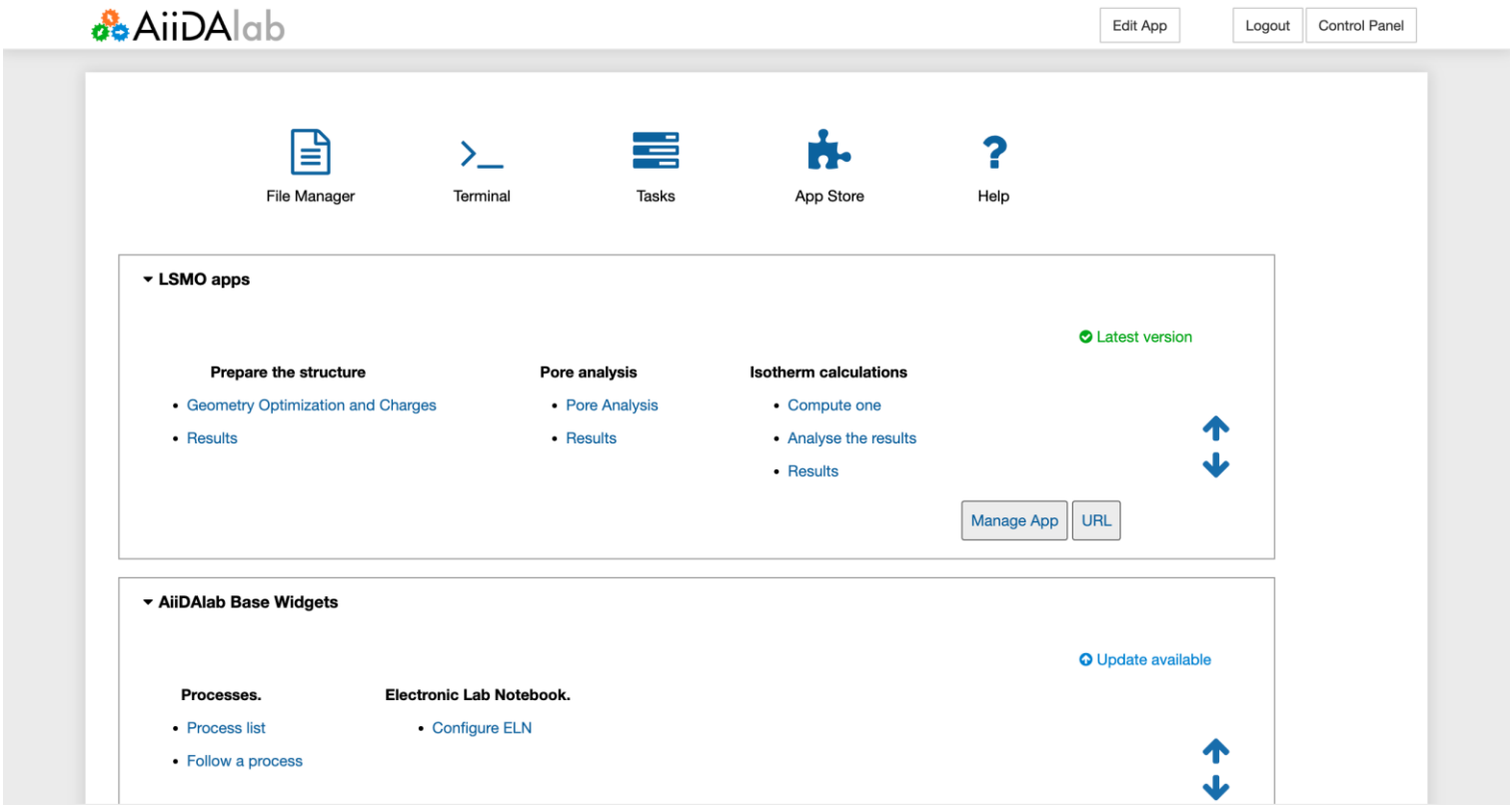


Requirements for MOFs



Geometry?
Chemistry?

How to measure?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Prepare the structure
Geometry Optimization and Charges
Results
Pore analysis
Pore Analysis
Results
Isotherm calculations
Compute one
Analyse the results
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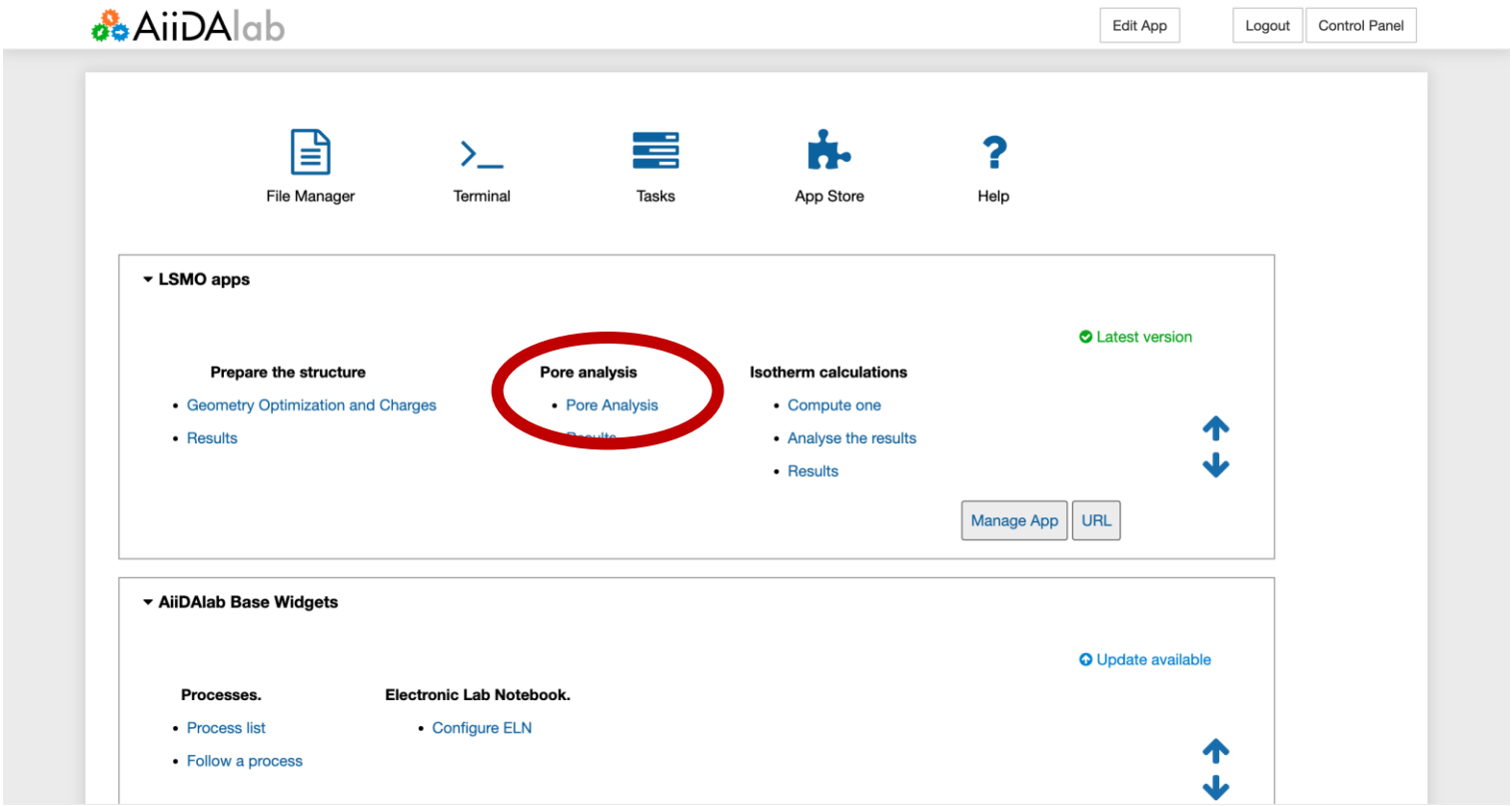
Processes.
Process list
Follow a process
Electronic Lab Notebook.
Configure ELN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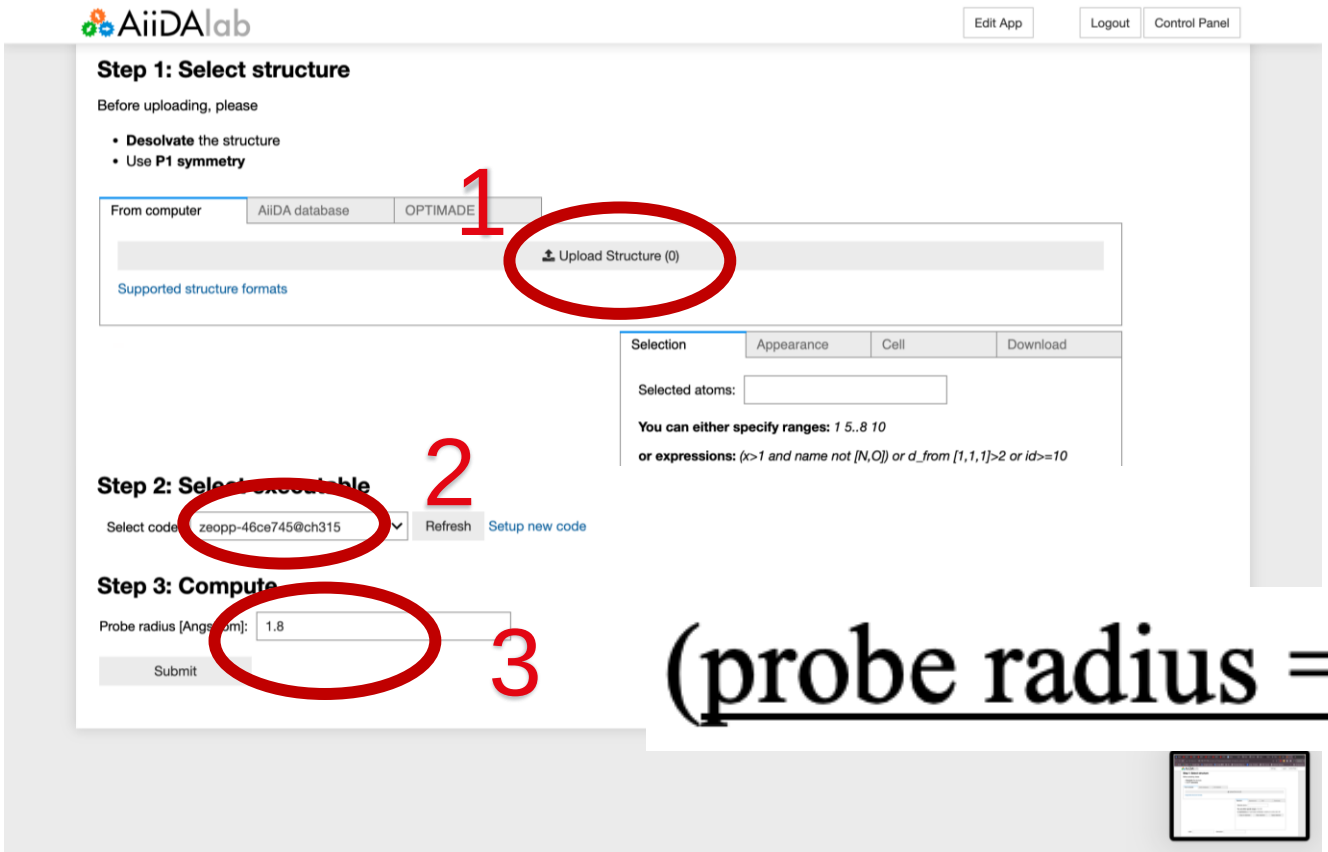
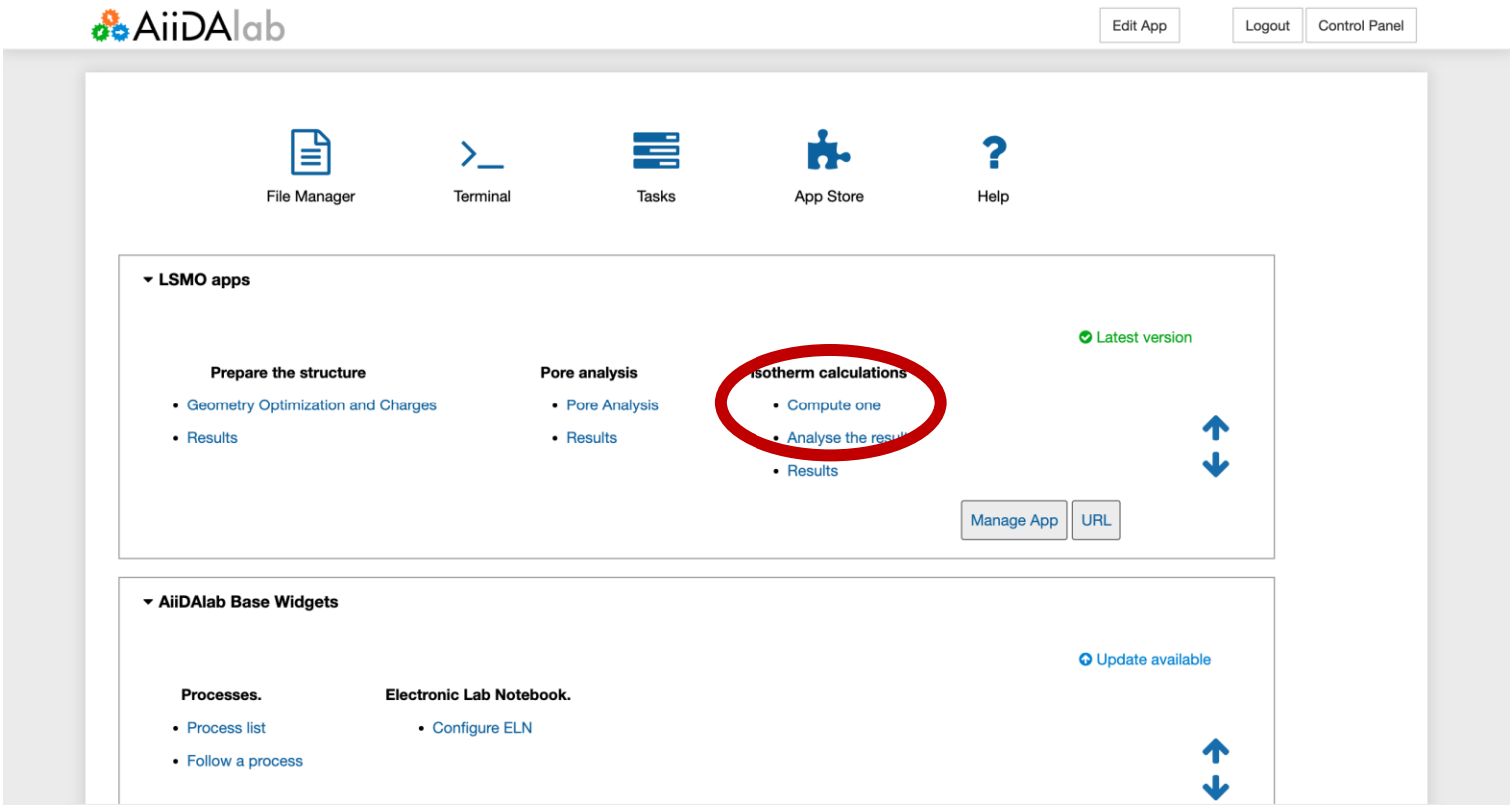


(probe radius = 1.525 Å)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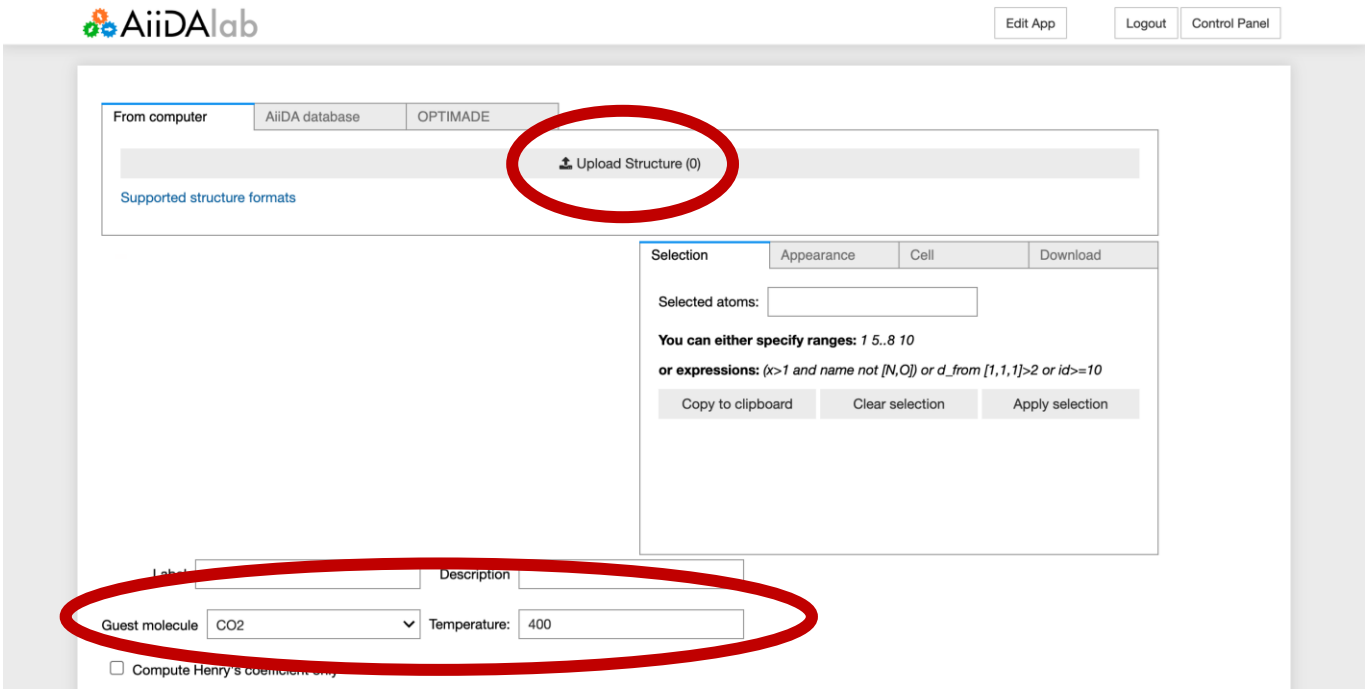
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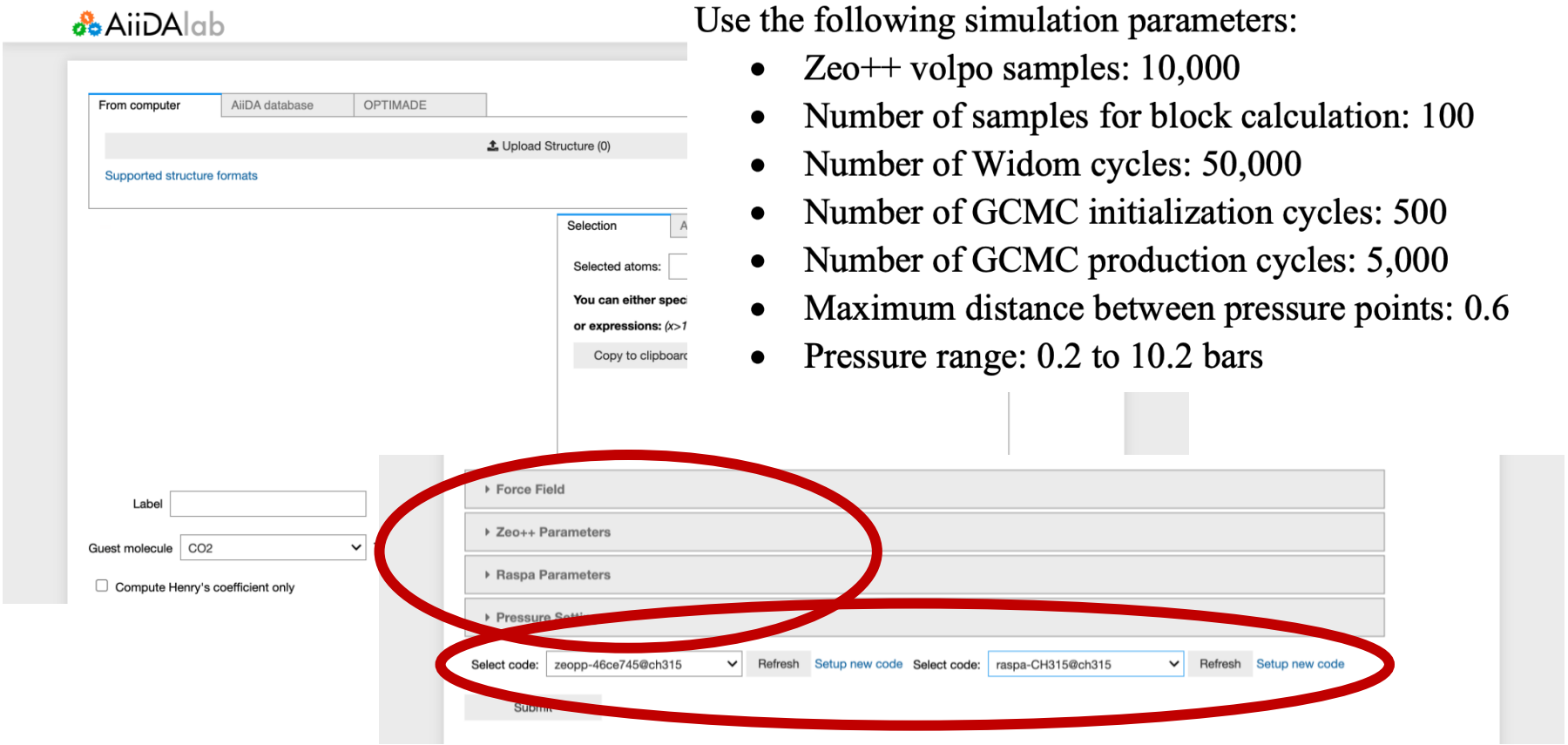
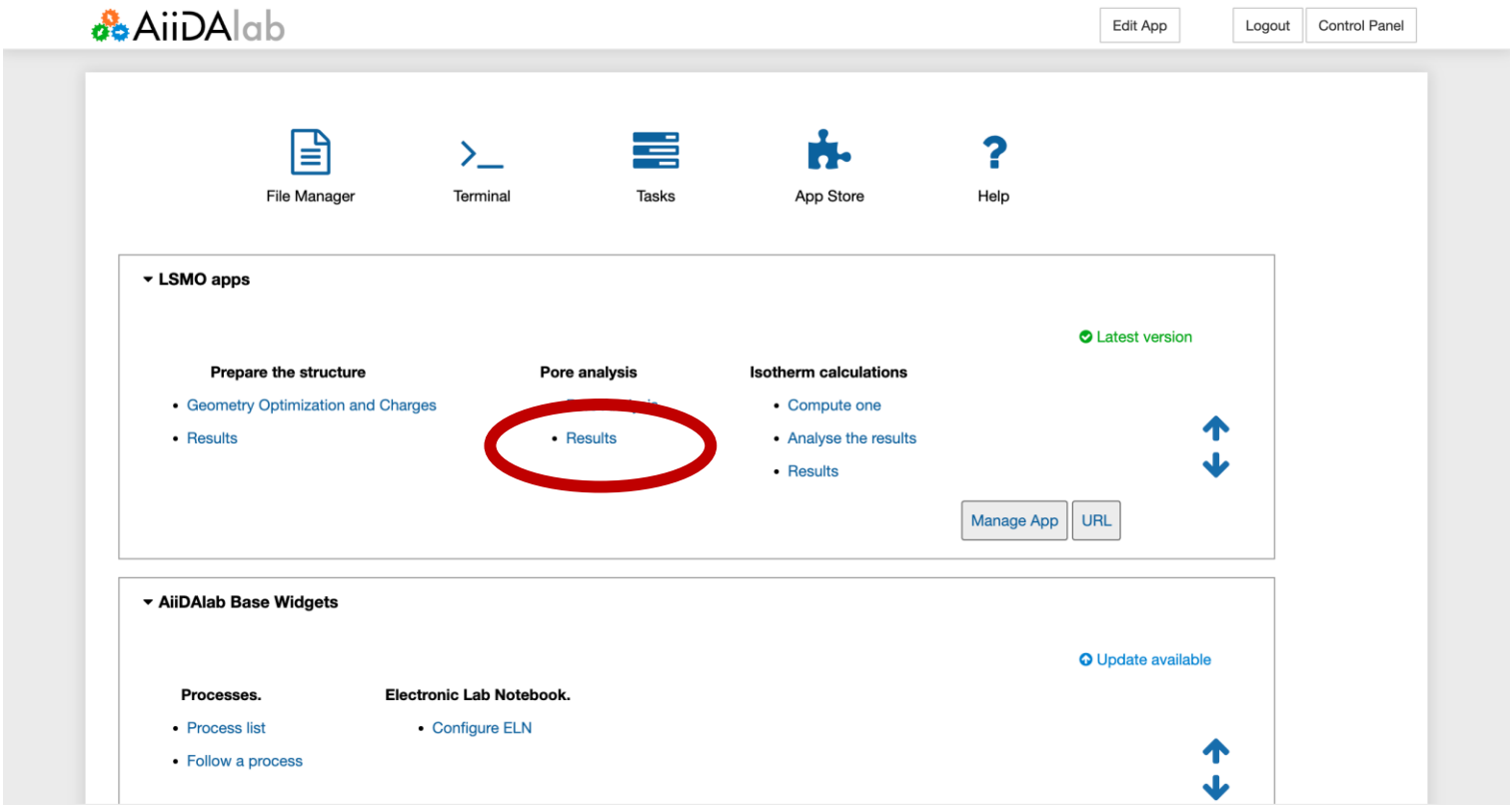
AiiDA database
OPTIMADE
Upload Structure (0)
Supported structure formats
Selection
Appearance
Cell
Download
Selected atoms:
You can either specify ranges: 1 5..8 10
or expressions: (x>1 and name not [N,O]) or d_from [1,1,1]>2 or id>=10
Copy to clipboard
Clear selection
Apply selection
Description
Guest molecule
CO2
Temperature:
400



Use the following simulation parameters:

- Zeo++ volpo samples: 10,000
- Number of samples for block calculation: 100
- Number of Widom cycles: 50,000
- Number of GCMC initialization cycles: 500
- Number of GCMC production cycles: 5,000
- Maximum distance between pressure points: 0.6
- Pressure range: 0.2 to 10.2 bars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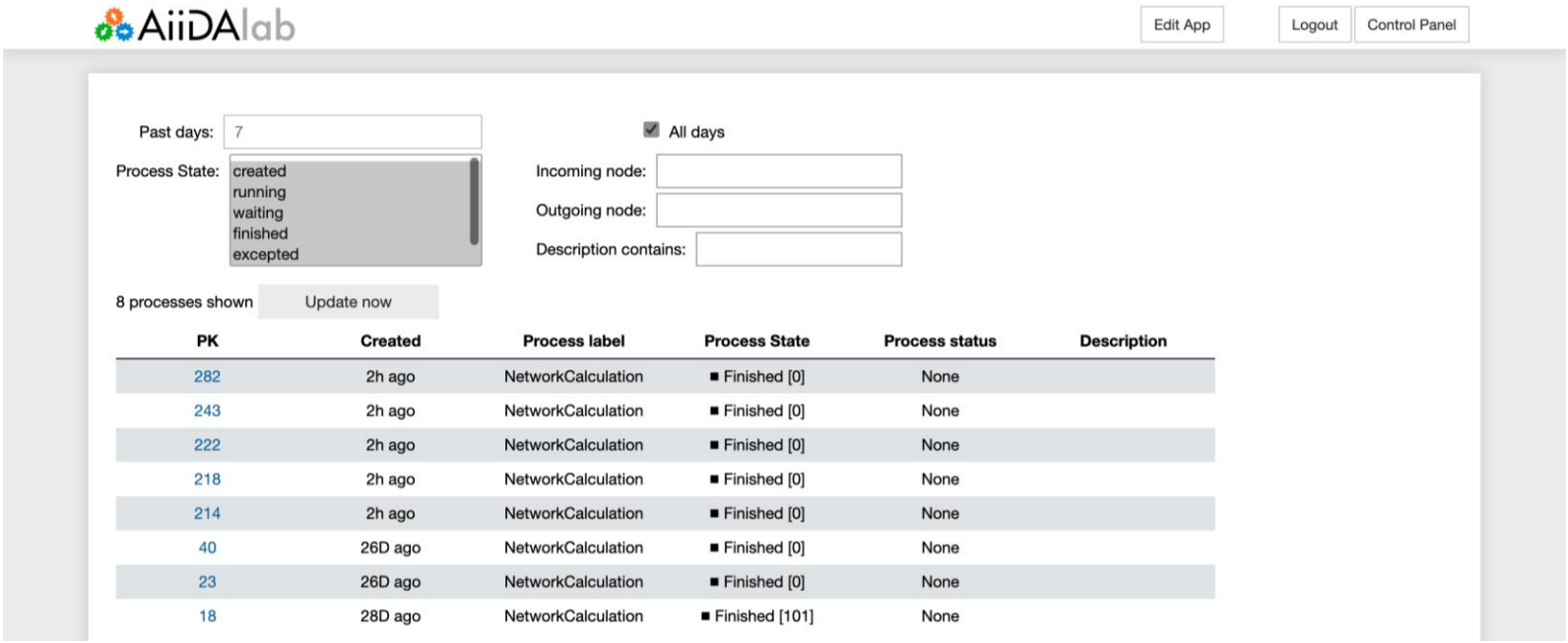
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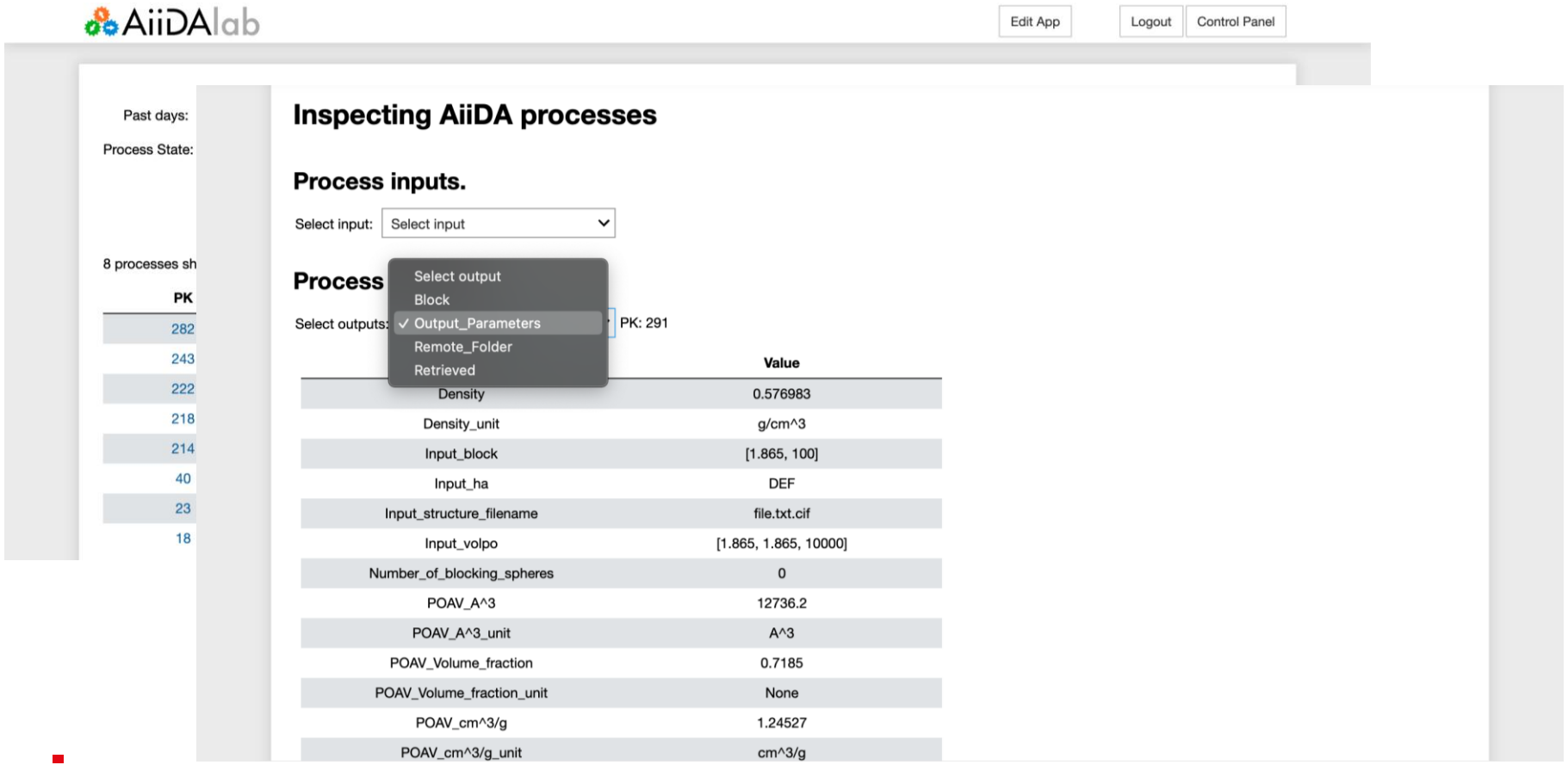
Past days: 7
All days
Process State: created running waiting finished excepted
Incoming node:
Outgoing node:
Description contains:
8 processes shown
Update now
PK Created Process label Process State Process status Description
282 2h ago NetworkCalculation ■ Finished [0] None
243 2h ago NetworkCalculation ■ Finished [0] None
222 2h ago NetworkCalculation ■ Finished [0] None
218 2h ago NetworkCalculation ■ Finished [0] None
214 2h ago NetworkCalculation ■ Finished [0] None
40 26D ago NetworkCalculation ■ Finished [0] None
23 26D ago NetworkCalculation ■ Finished [0] None
18 28D ago NetworkCalculation ■ Finished [101] None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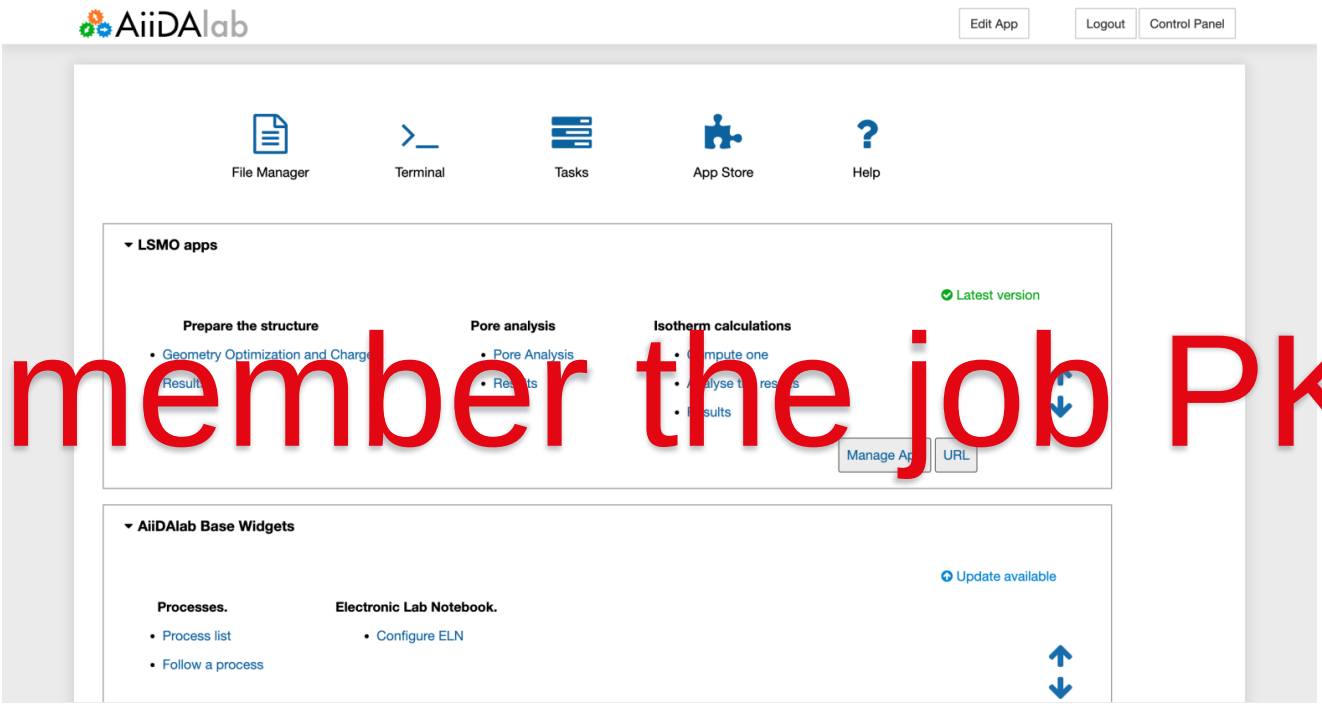
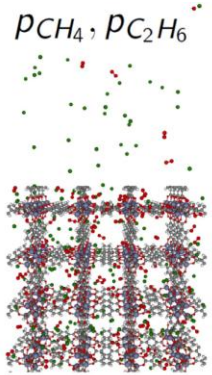
Past days:
Process State:
8 processes sh
PK
282
243
222
218
214
40
23
18
Inspecting AiiDA processes
Process inputs.
Select input:
Select input
Process
Select outputs:
Select output
Block
Output_Parameters
Remote_Folder
Retrieved
PK: 291
Value
Density
0.576983
Density_unit
g/cm^3
Input_block
[1.865, 100]
Input_ha
DEF
Input_structure_filename
file.txt.cif
Input_volpo
[1.865, 1.865, 10000]
Number_of_blocking_spheres
0
POAV_A^3
12736.2
POAV_A^3_unit
A^3
POAV_Volume_fraction
0.7185
POAV_Volume_fraction_unit
None
POAV_cm^3/g
1.24527
POAV_cm^3/g_unit
cm^3/g



Remember the job PKs!!!

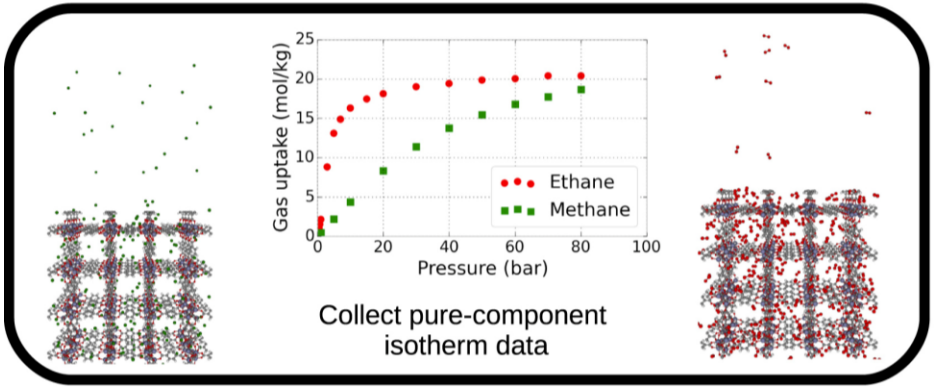
For more info on AiiDA look at: https://www.aiida.net/

Ideal Adsorption Solution Theory (IAST)



Goal: predict a mixed gas adsorption isotherm

Example: methane/ethane in IRMOF-1

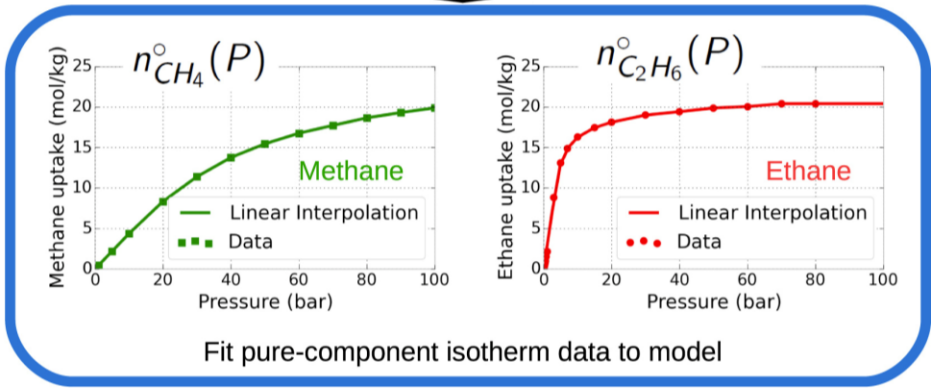


$$\pi_{CH_4}(p^\circ_{CH_4}) = \pi_{C_2H_6}(p^\circ_{C_2H_6})$$
$$p_{CH_4} = x_{CH_4} p^\circ_{CH_4}$$
$$p_{C_2H_6} = x_{C_2H_6} p^\circ_{C_2H_6}$$
$$x_{CH_4} + x_{C_2H_6} = 1$$

Solve for adsorbed phase composition

$$\frac{1}{n_{CH_4}+n_{C_2H_6}} = \frac{x_{CH_4}}{n^\circ_{CH_4}(p^\circ_{CH_4})} + \frac{x_{C_2H_6}}{n^\circ_{C_2H_6}(p^\circ_{C_2H_6})}$$

Solve for total gas adsorbed



- https://doi.org/10.1016/j.cpc.2015.11.016

Evaluation of IRMOF-1