MOFLearning : Streamlined Simulation Workflows for Gas Adsorption in Metal-Organic Frameworks

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Abstract

Metal-Organic frameworks (MOFs) known for their high porosity and structural tunability, are promising for gas storage, separations, and catalysis applications.

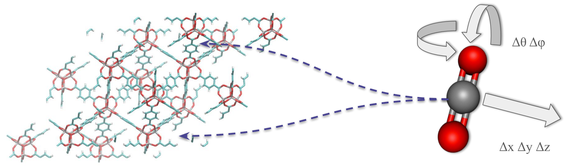
The experimental Cambridge Structural Database (CSD) or other **ready-to-use structural databases** (e.g. CoRE-MOFs, ARCMOF) facilitates **property characterization** through molecular simulations, covering adsorption, thermal, mechanical, and electronic properties.

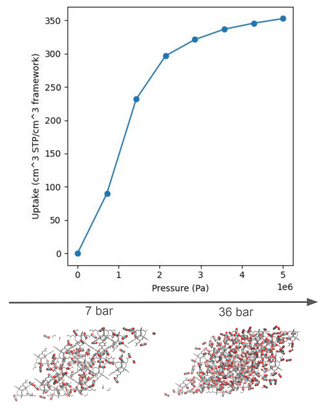
However, simulation tools often require **advanced expertise**, and although many computational codes are accessible, they remain time-consuming and challenging for non-expert users.

The DIAMOND project (PEPR DIADEM) promotes **FAIR data practices** with reproducible, **user-friendly workflows** using workflow managers (e.g. AiiDA) and containerization. We present such an easy-to-use pipeline for simulating adsorption properties of polar gases (e.g., N_2, CO_2) in MOFs, streamlining advanced analyses across platforms.

Gas Adsorption in MOFs

Grand Canonical Monte Carlo (GCMC) simulation is a computational technique that models gas adsorption in porous materials like MOFs by allowing the number of gas molecules to fluctuate within a fixed volume, temperature, and chemical potential to reach equilibrium. GCMC accurately predicts **adsorption capacities**, **selectivity** and other thermodynamic properties.



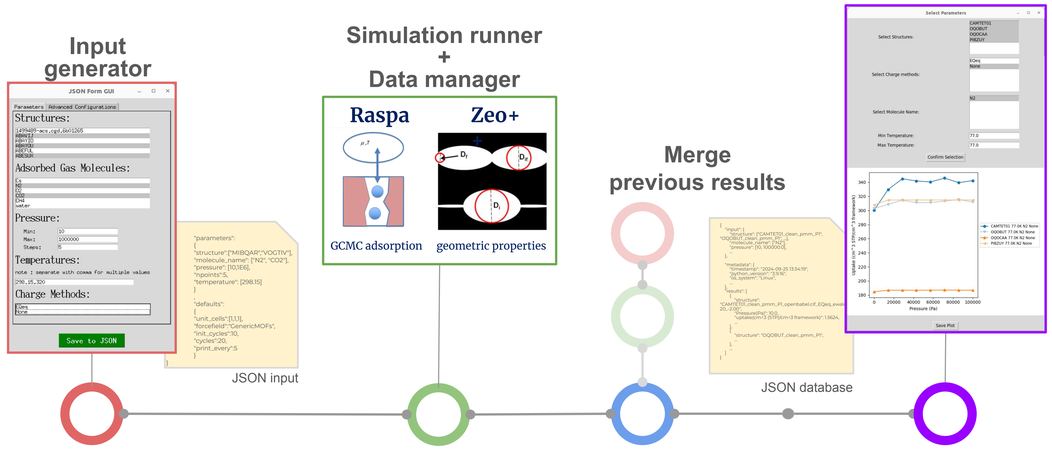


A FAIR workflow

simple-adsorption-workflow

- A python workflow using input/output **JSON files**
- **User-friendly interfaces**
- Tested on Gricad/dahu and Idris/Jean-zay **HPC**
  - single CPU simulations
  - parallelization on materials/conditions/properties
- Inputs from structural databases (Core MOF 2019)
- A fully **containerized** package

```
$ apptainer run simple-adsorption-workflow.sif   input
$  ...                                           run
$  ...                                           merge
$  ...                                           plot
```



Benchmark on HPC

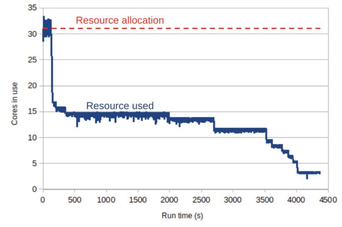
Portable Apptainer image

↓

Test on Dahu (Gricad)

- The workflow **performances** with the apptainer image in the HPC cluster are **similar** to the ones observed with a standard installation (conda)
- But the **GCMC calculation time** is :
  - **not easily predictable**
  - system/model dependent

⇨ Low efficiency (CPU usage vs. allocation)



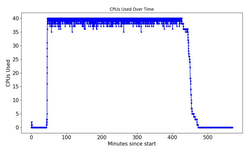
128 simulations
4 Nodes
32 cpus/node

4 materials
2 charge methods
2 gases
8 pressure points

Ongoing developments

New features

- Add input keywords from individual codes
- Screening requirements
  - user warnings
  - internal scheduler
  - other MOF databases



CPU maximal efficiency for a batch of single-simulations (EQeq charges calculations) with heterogeneous time durations

Advanced Workflows for screening

AiiDA

RASPA3

aiida-adsorption-wf

Extension of the adsorption workflow integrating AiiDA

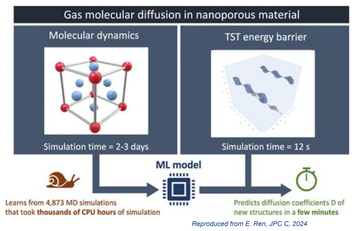
LAMMPS

aiida-diffusion-wf

Compute self-diffusion of gas adsorbates in porous materials

Long-term

- Provide systematic theoretical **support for adsorption experiments**
- Screen the **CoRE-MOF 2019** database for **diffusion coefficients** of polar gases
- **Predict properties** using ML models



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