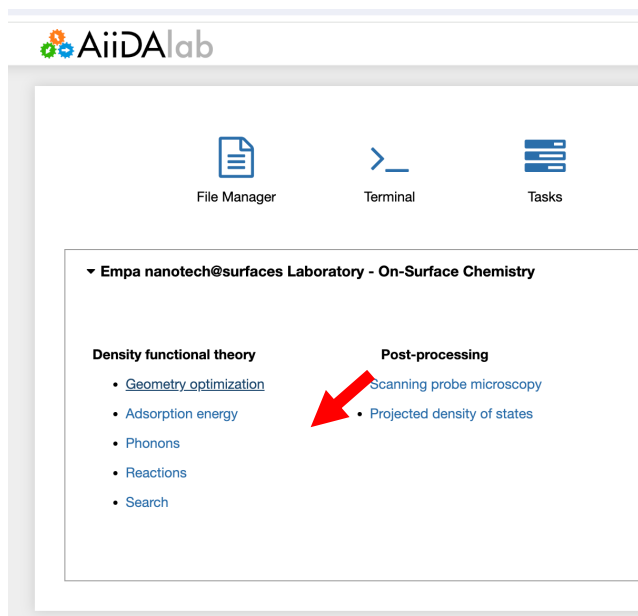
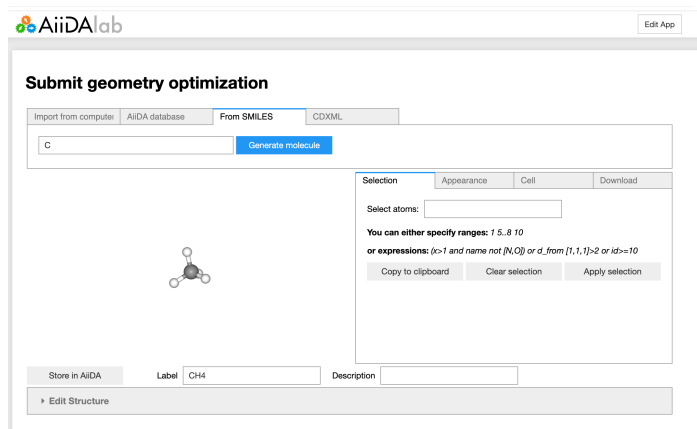


Setting up a «computer» on piz daint (CSCS Lugano)

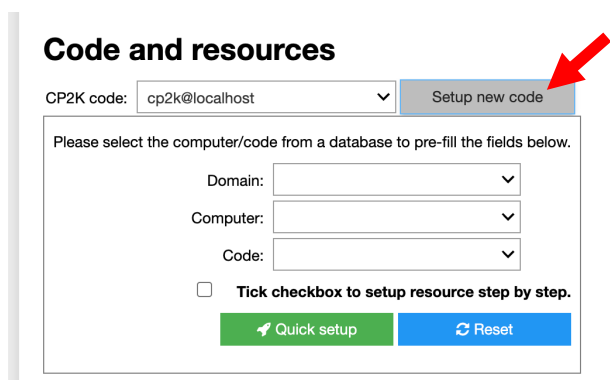
Start with clicking on “Submit geometry optimization”



Insert any molecule (e.g. SMILES for methane)



Scroll down to “Code and resources”, hit “**setup new code**”



Give the following parameters (including the course account name you got per E-Mail, and hit “Quick Setup”

Code and resources

CP2K code:

Please select the computer/code from a database to pre-fill the fields below.

Domain:

Computer:

Code:

[Piz Daint](#) supercomputer at CSCS Lugano, Switzerland, hybrid partition.

The CSCS now require MFA to login, please check the [MFA CSCS documentation](#) for details on how to set up SSH connection.

If you are using the AiiDALab, [use the MFA CSCS app](#) to set SSH connection.

Computer Label:

Slurm account:

Slurm partition:

Multithreading hint:

Setup up the SSH connection.

SSH username:

☐ Tick checkbox to setup resource step by step.

At this point, go to the “Exercise9” directory and give the command:

“./initialize_daint.sh”

This will copy the private key to your ~/.ssh directory .

The public key of your account courseXX (with XX=01—30) is already on the supercomputer.

Go to a terminal and give the command

➤ `ssh daint.cscs.ch`

if it connects to daint without password, **very good!** Hit “exit” and go back to your shell.

If not, give the command

➤ `ssh-copy-id daint.cscs.ch`

and give the password you got by email as many times as requested.

Then try

➤ `ssh daint.cscs.ch`

You will be requested the password, exit then daint and repeat until the password is not requested anymore.

The content of the file ~/.ssh/config is:

```
(base) jovyan@d633c698dc55:~$ more .ssh/config
```

```
Host daint.cscs.ch
```

```
User course18
```

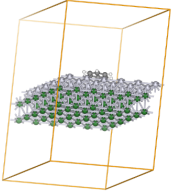
```
Port 22
```

```
ProxyCommand ssh -q -Y course14@ela.cscs.ch netcat daint.cscs.ch 22
```

```
ServerAliveInterval 5
```

Now, when you want to start a geo opt on daint, select the corresponding computer/code as in the following figure:

PK- 403 | 2024-04-23 22:25 | C6H6Pt108 | StructureData |



Selection

Appearance

Cell

Download

Select atoms: 1..72

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

Selected atoms: 1..72

Selected unit cell atoms: 1..72

Geometric center: (12.7 7.6 11.13)

72 atoms selected

Store in AiiDA

Label

Description

Edit Structure

Inputs

☒ Dispersion Corrections

Spin-polarized calculation

Structure details

Constraint fixed xyz 1..72

Add constraint

Remove constraint

Show help

Protocol: Low accuracy

Code and resources

CP2K code: cp2k-9.1@dsaint-gpu

Setup new code

Nodes4

Tasks per node12

Threads per task1

Walltime: 24:00:00

Walltime will be: 1 days 00:00:00

Estimate resources

Submit

Workflow description: benzene 3 layers

Submit