FireWorks for Materials Science

HPC Workflow

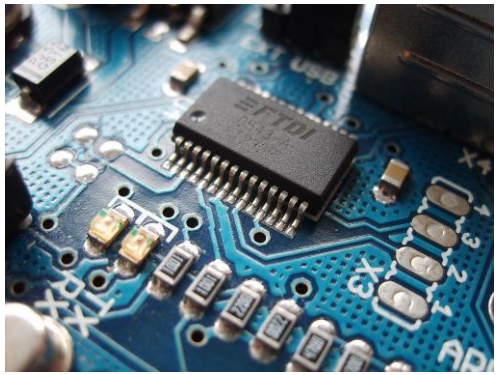
Guillaume Brunin

February 16, 2022

UCLouvain

Institute of Condensed Matter and Nanosciences

Functional materials are used in many applications every day



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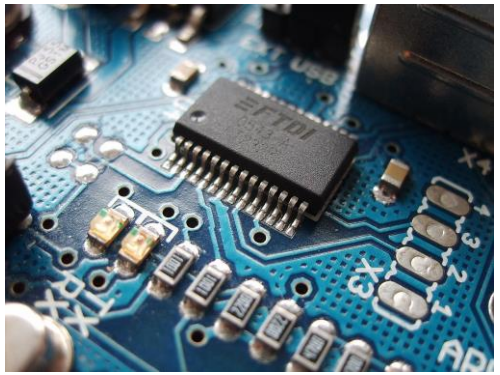

- Better materials for PV ?

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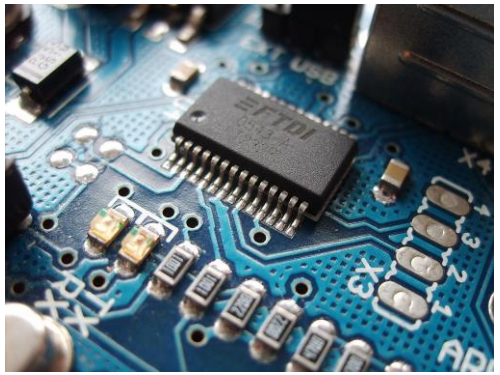

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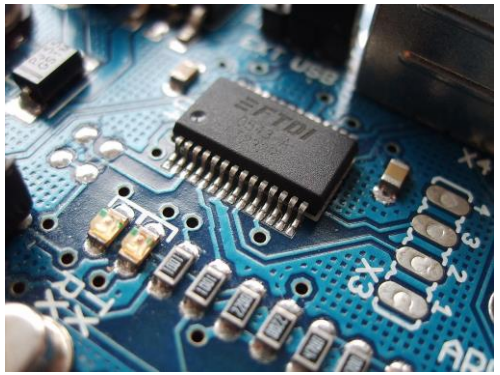

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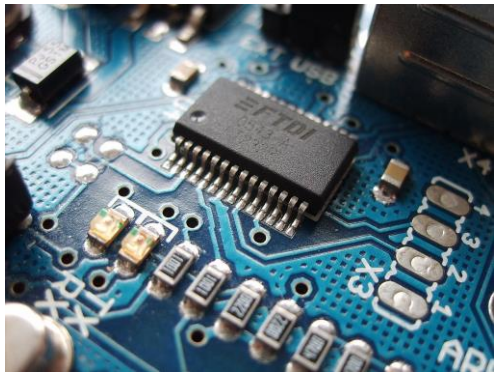

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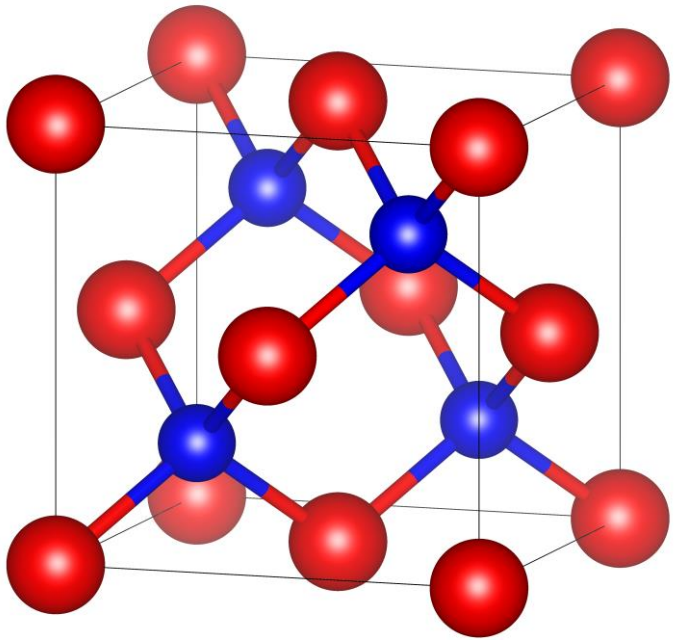
- Better energy storage ?

Computational predictions can help finding good new materials...



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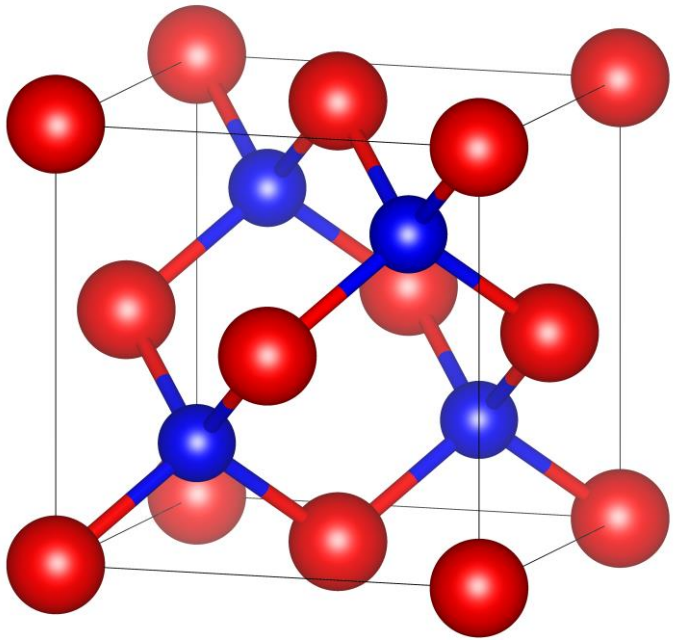

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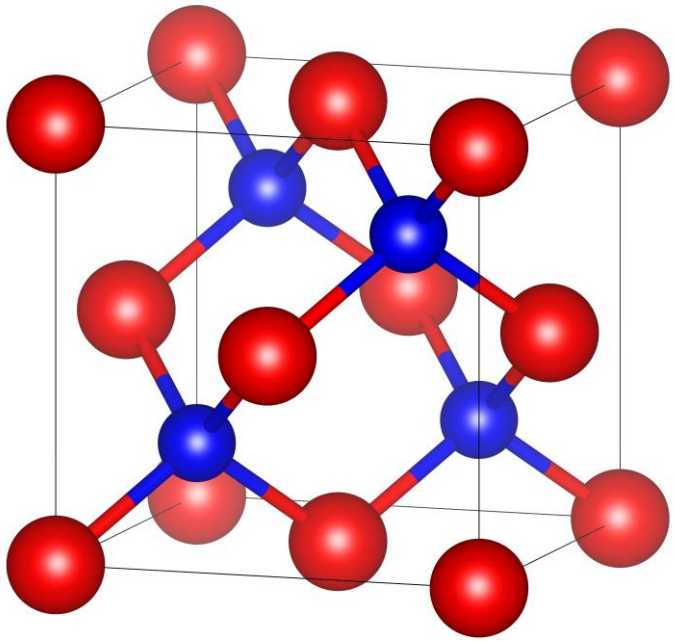

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- Thermodynamics, phase diagrams
- Electronic structure
- Transport (heat, electricity)
- Vibrational properties
- Magnetic properties
- Defect concentration
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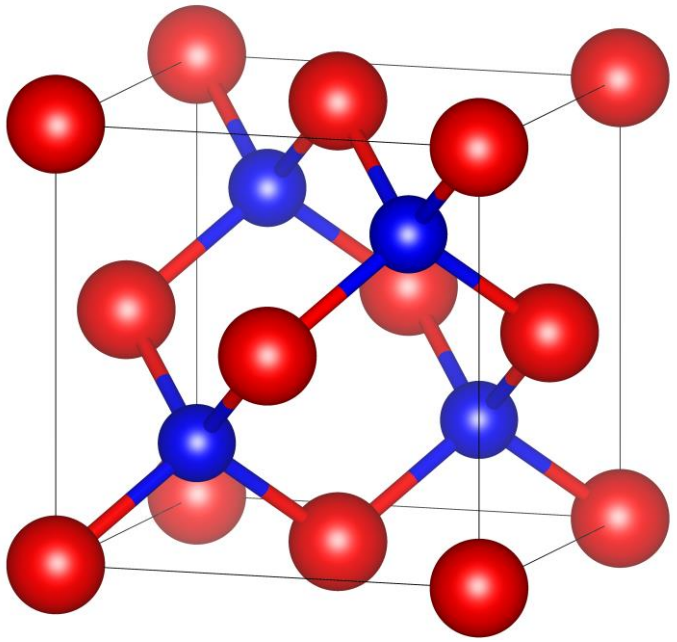

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Each of these properties requires from 1 to 10's of different computations

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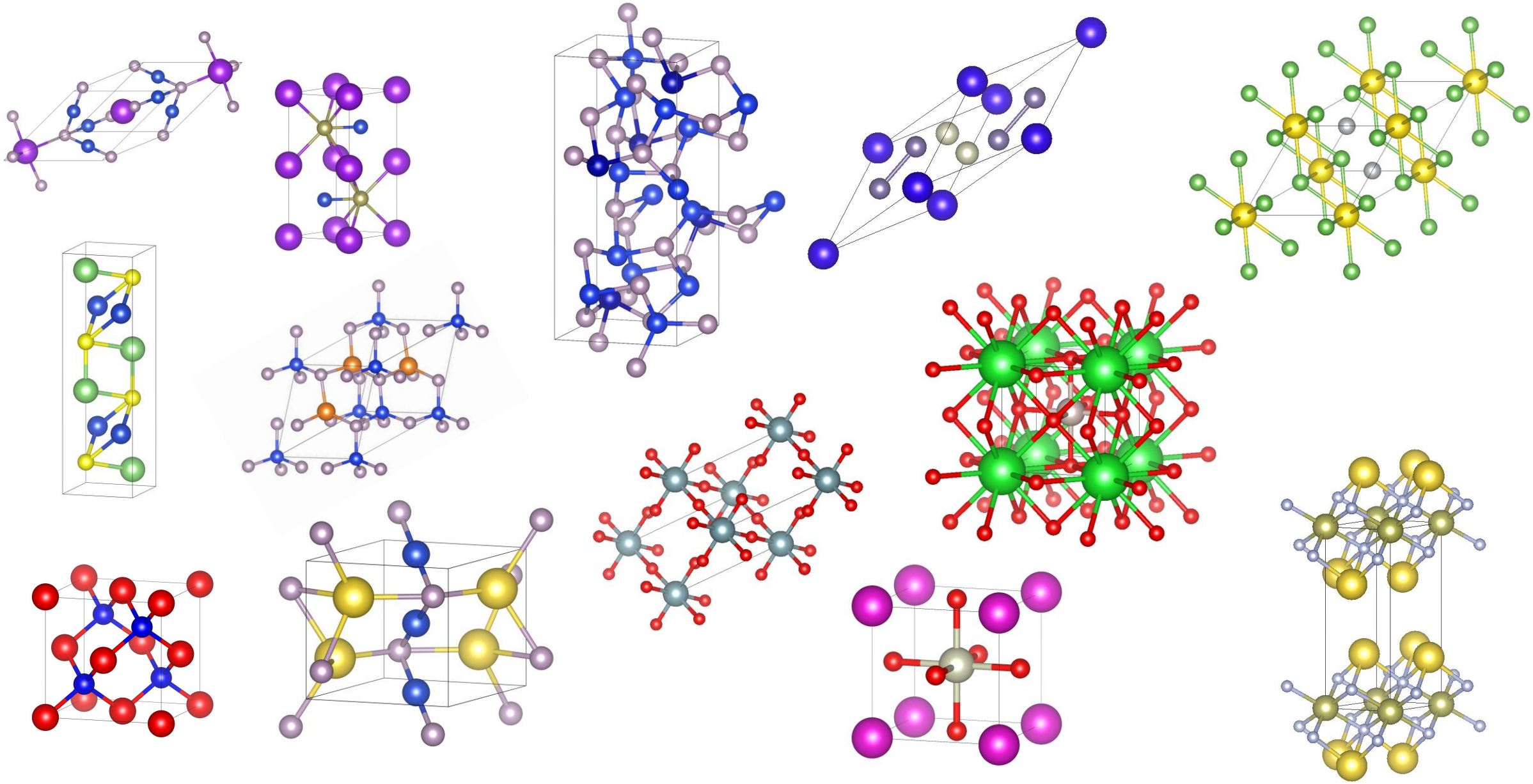

Instead of hiring an army of students, we can automate things

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VS

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pymatgen

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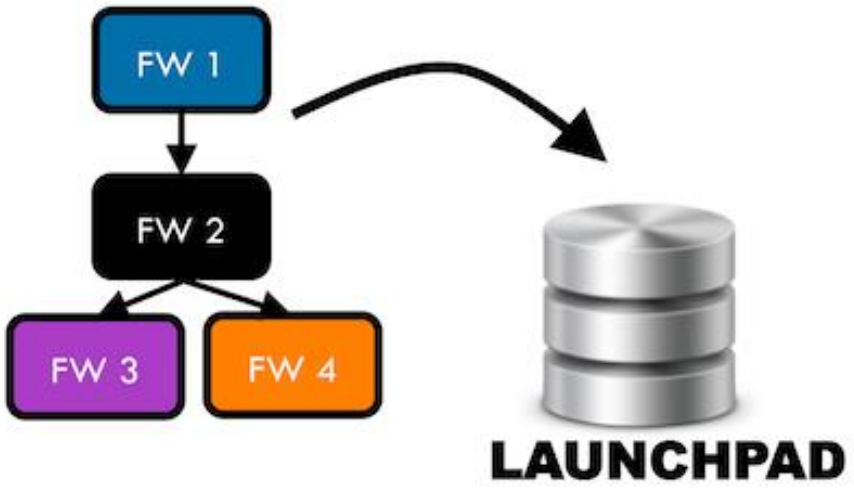
- Support for dynamic workflows
- Web GUI monitor

FireWorks is based on a centralized server



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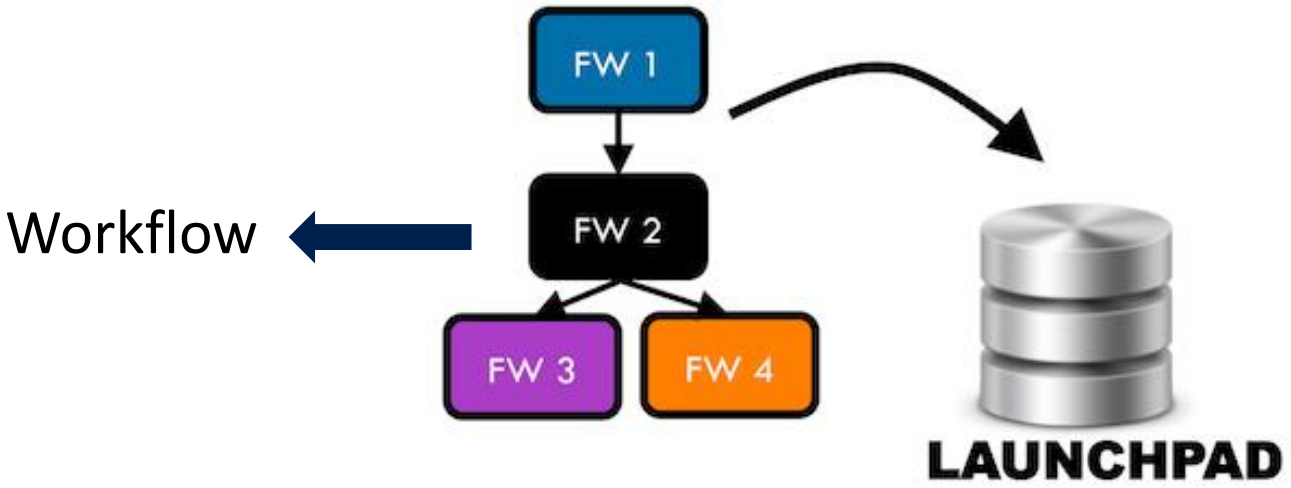

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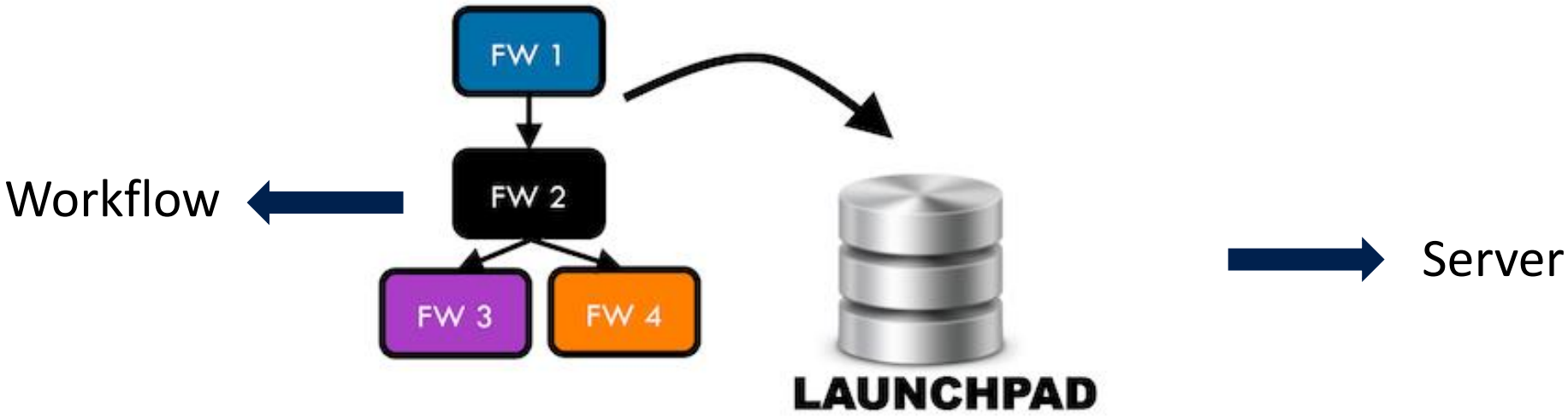

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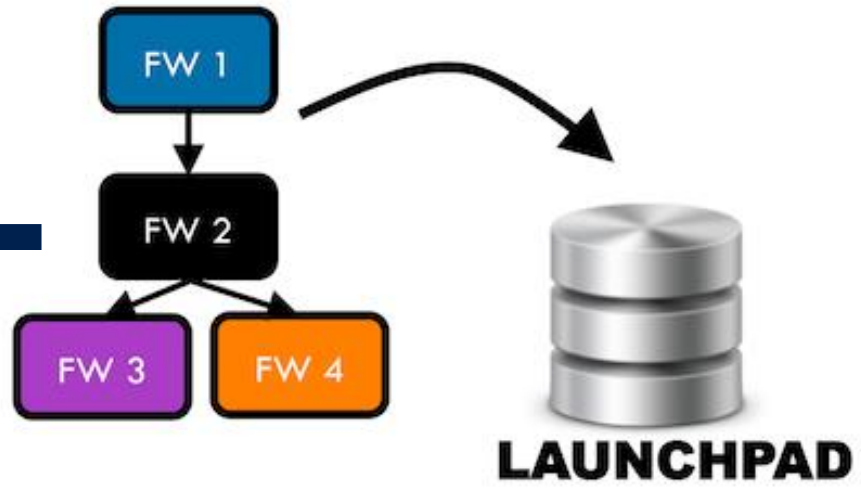
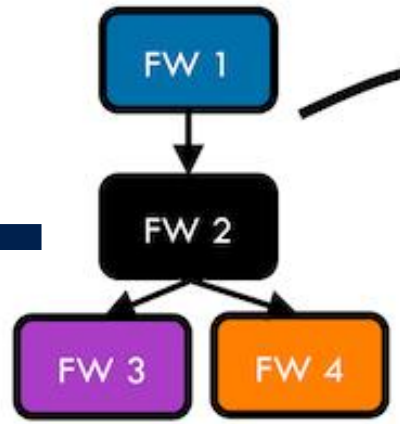
Workflow



Server : interface with the FW DB

FireWorks is based on a centralized server and on workers



Workflow

LAUNCHPAD

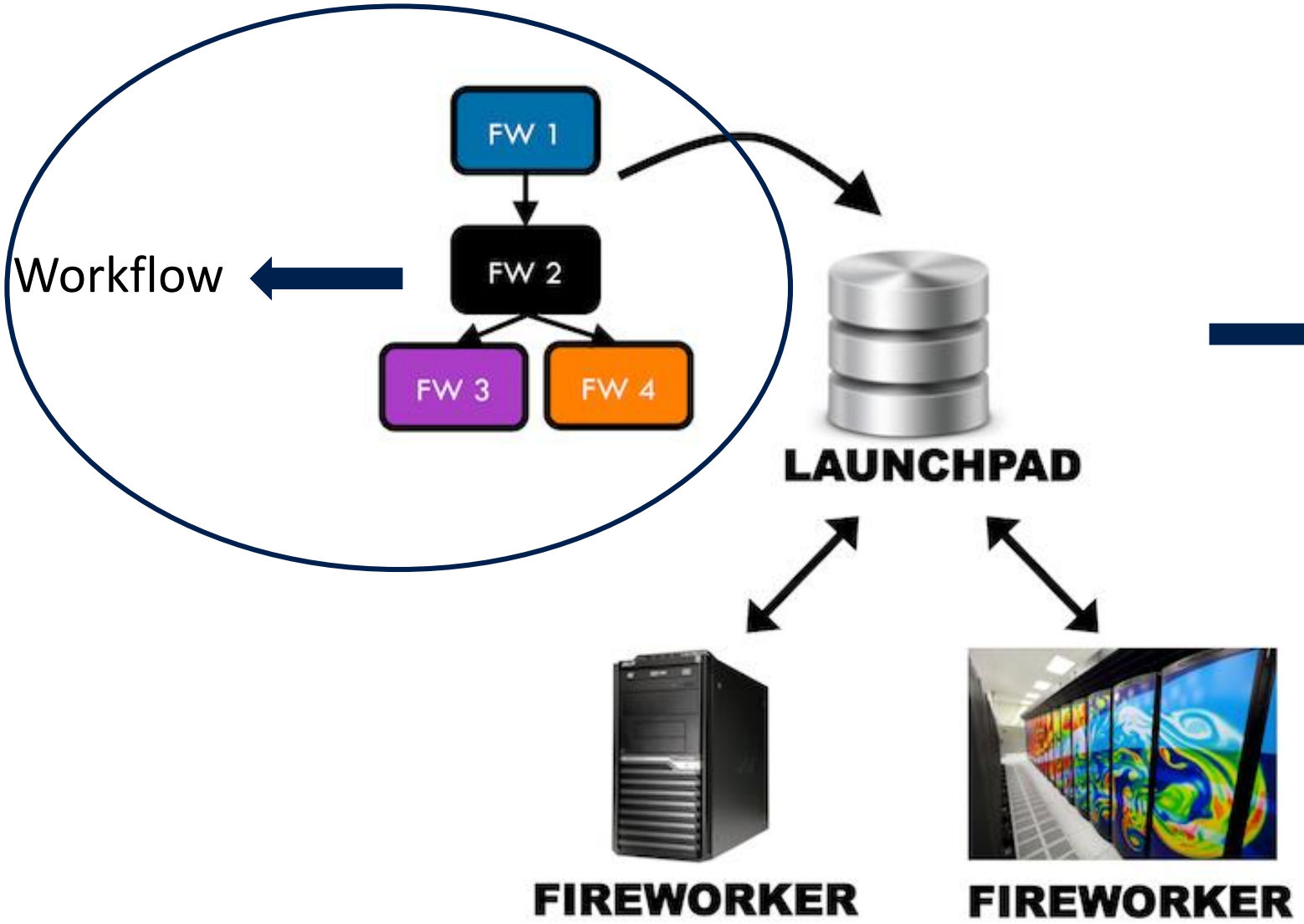
Server : interface with the FW DB

FIREWORKER

FIREWORKER

Workers : 1) execute the WF
2) stores the results in a DB

Let’s look a bit closer at how WF are defined in FireWorks



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A FireWorks WF is composed of basic building units

- Firework : list of tasks to be performed
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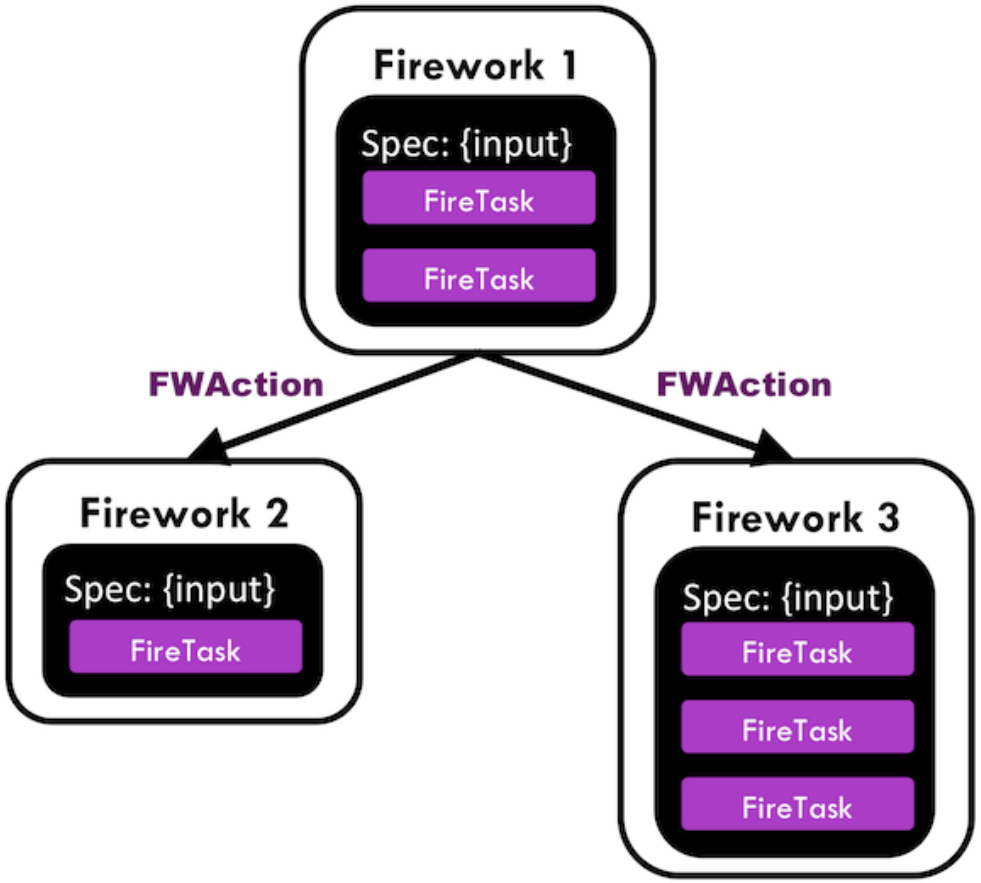

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- FireTask : atomic computing job
  (shell/python script, computation,
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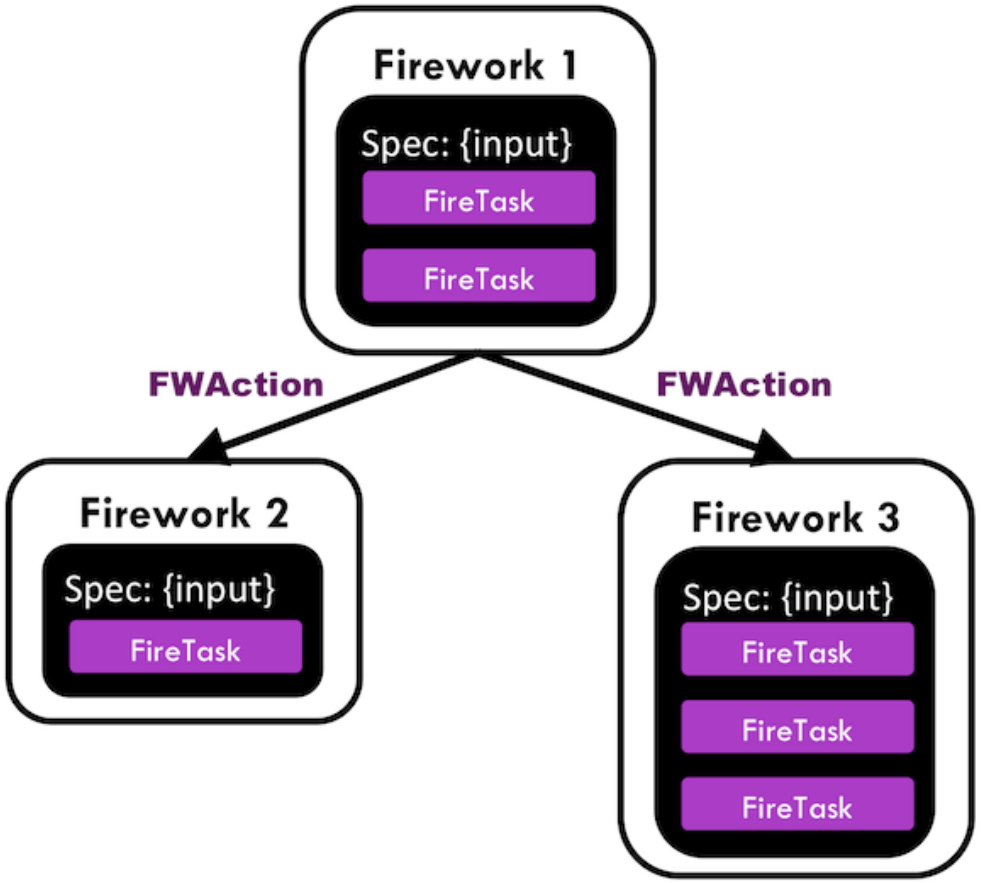

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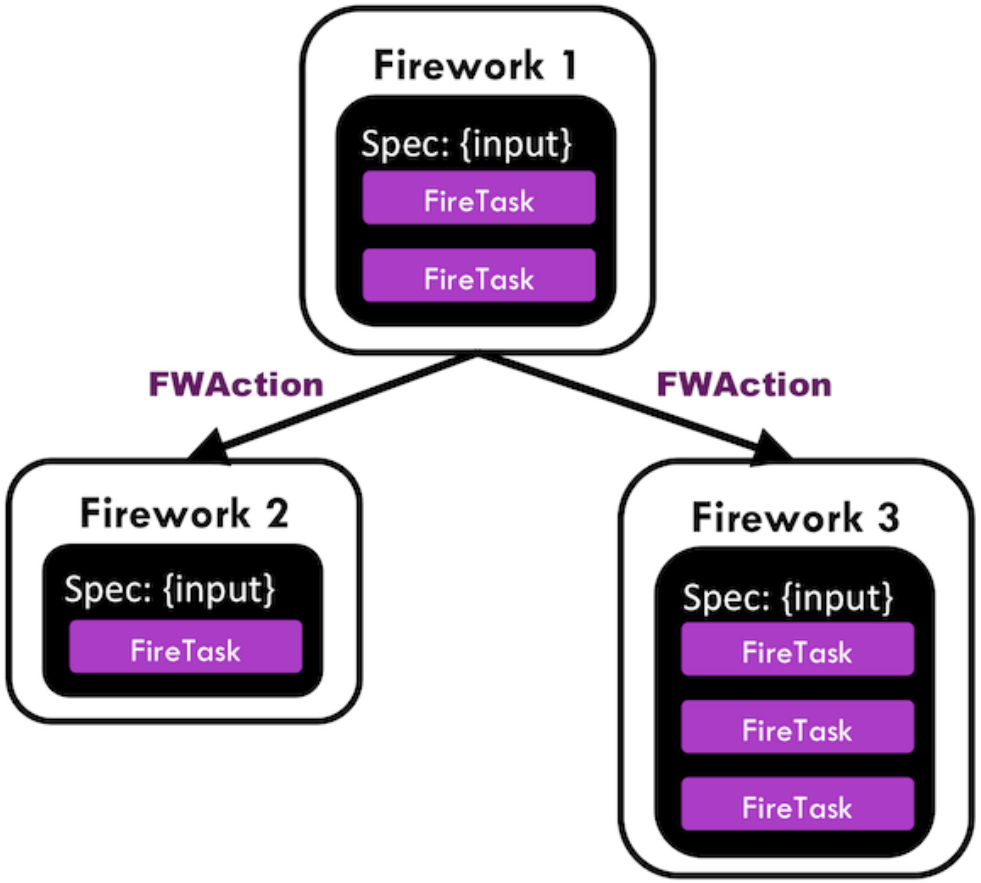
- FWAction : object returned at the end of each
  FireTask

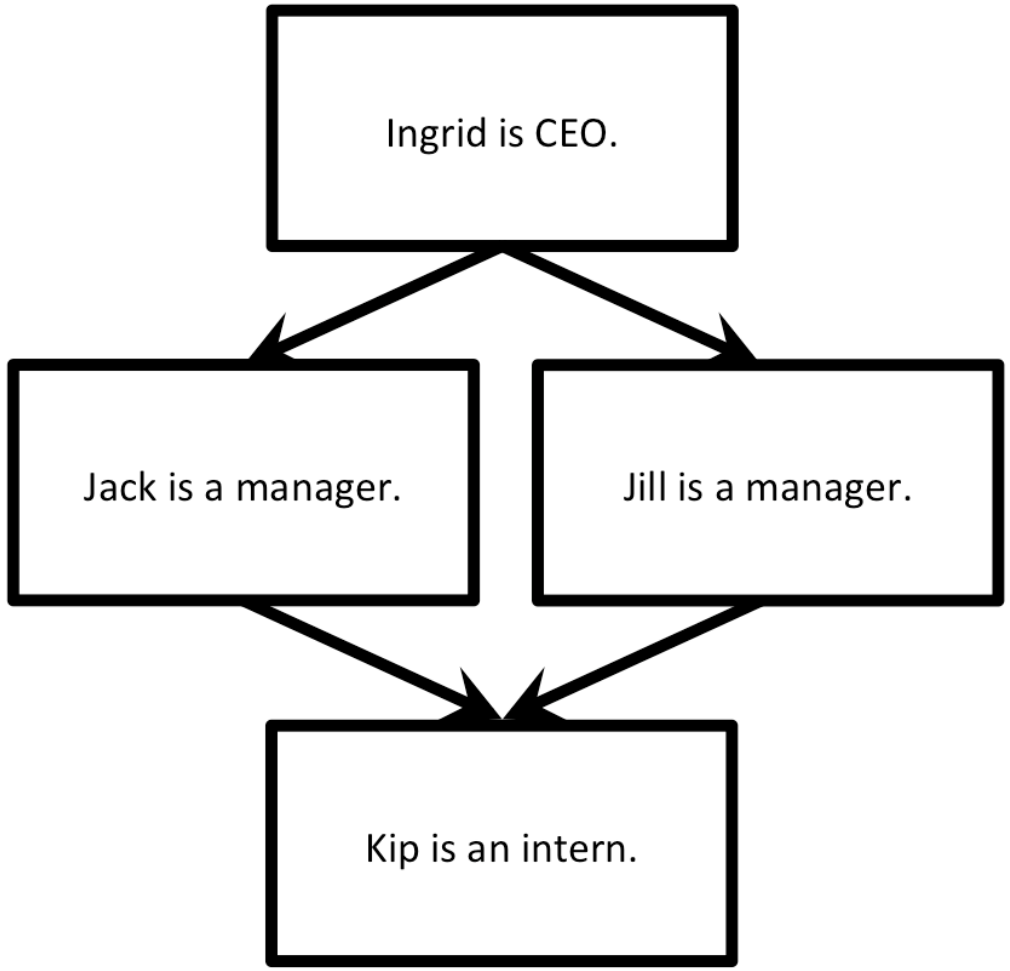


Let’s see a super simple example of a Workflow

```
# define four individual FireWorks used in the Workflow
task1 = ScriptTask.from_str('echo "Ingrid is the CEO."')
task2 = ScriptTask.from_str('echo "Jill is a manager."')
task3 = ScriptTask.from_str('echo "Jack is a manager."')
task4 = ScriptTask.from_str('echo "Kip is an intern."')

fw1 = Firework(task1)
fw2 = Firework(task2)
fw3 = Firework(task3)
fw4 = Firework(task4)

# assemble Workflow from FireWorks and their connections
workflow = Workflow([fw1, fw2, fw3, fw4],
                    {fw1: [fw2, fw3], fw2: [fw4], fw3: [fw4]})
```



Once the WF is added to the DB, we can tell FireWorks to start running

```
$ qlaunch rapidfire --nlaunches 1
INFO getting queue adapter
INFO Found previous block, usingblock_2019-02-04-16-25-31-583641
INFO The number of jobs currently in the queue is: 0
INFO 0 jobs in queue. Maximum allowed by user: 0
INFO Launching a rocket!
INFO Created new dir block_2019-02-04-16-25-31-583641/launcher_2019-02-04-16-27-54-081986
INFO moving to launch_dir block_2019-02-04-16-25-31-583641/launcher_2019-02-04-16-27-54-081986
INFO submitting queue script
INFO Job submission was successful and job_id is 5
INFO Launched allowed number of jobs: 1
```

We can monitor what is happening using a GUI

FireWorks

Newest Workflows

CompanyStructure READY ID: 3088

AssignJob
AssignJob
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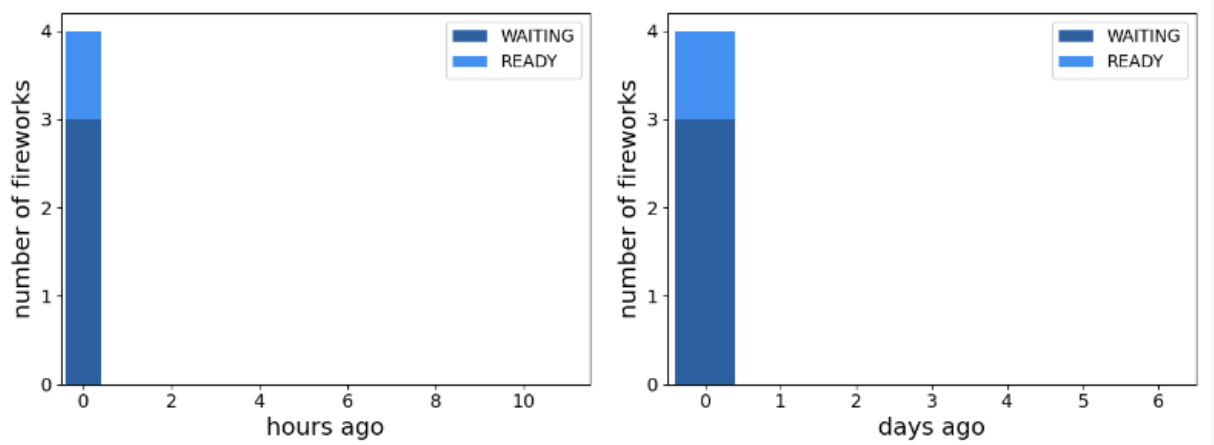

Database snapshot

	Fireworks	Workflows

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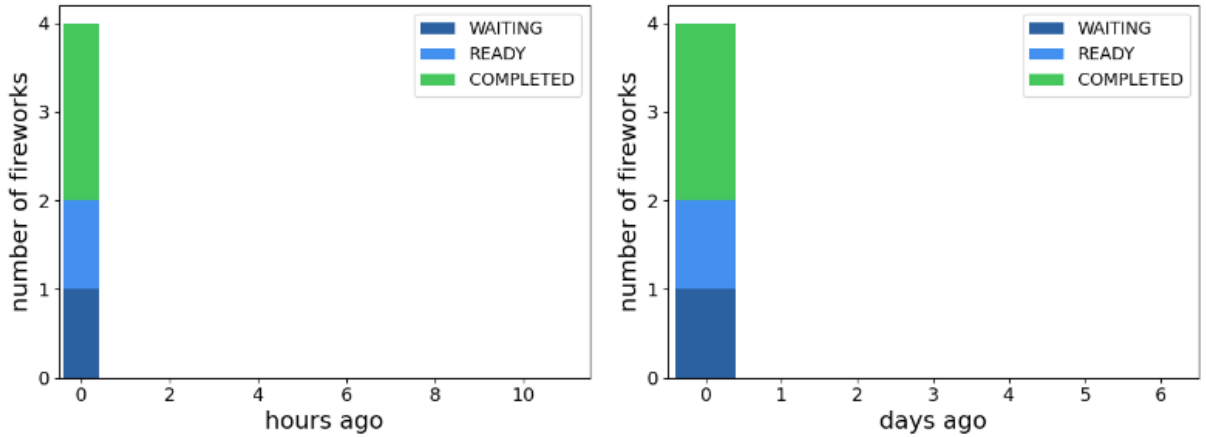

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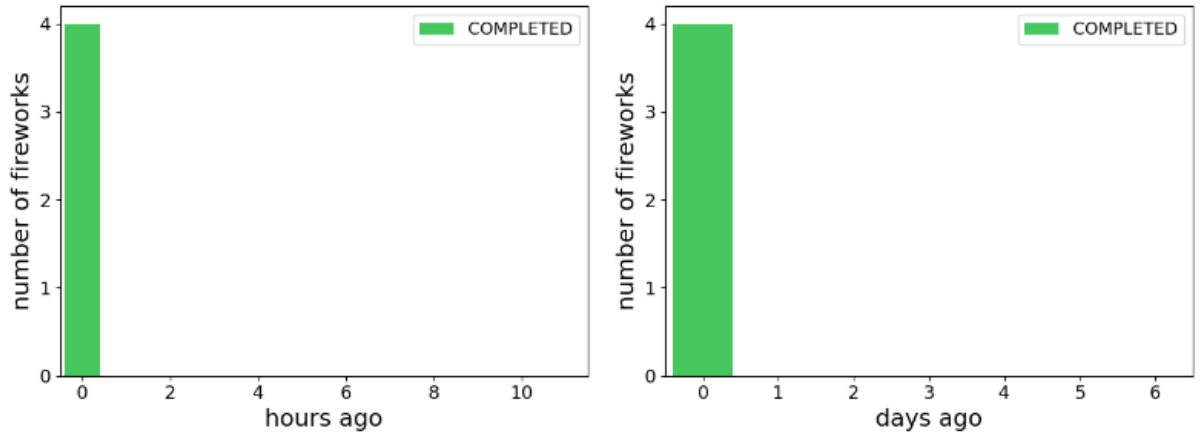

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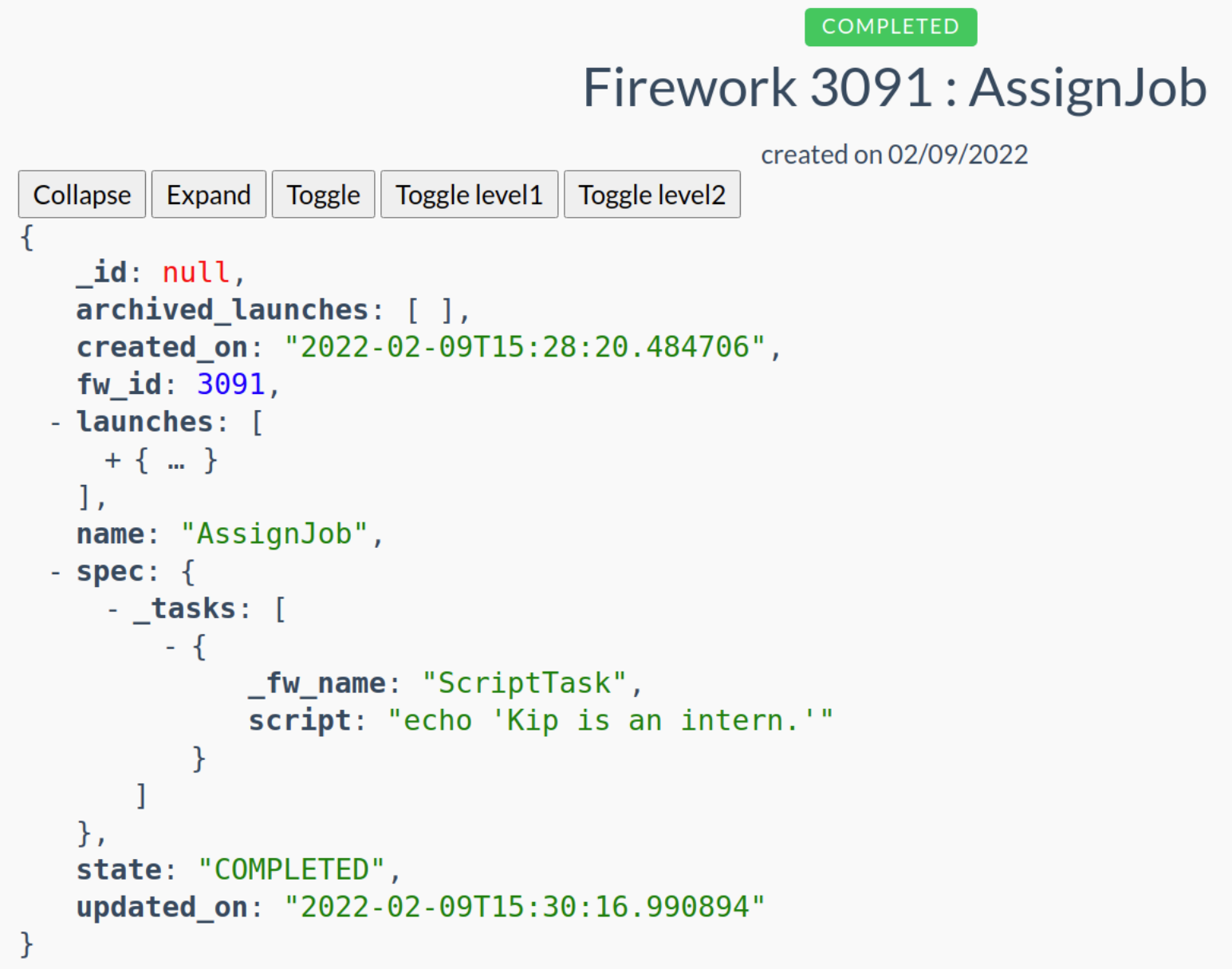

This is just a very superficial introduction !

The tutorials are very useful and the website well documented

- FireWorks documentation :

https://materialsproject.github.io/fireworks/

- Paper :

“FireWorks: a dynamic workflow system designed for high-throughput applications”. Concurr. Comput. Pract. Exp. 22, 5037–5059 (2015)

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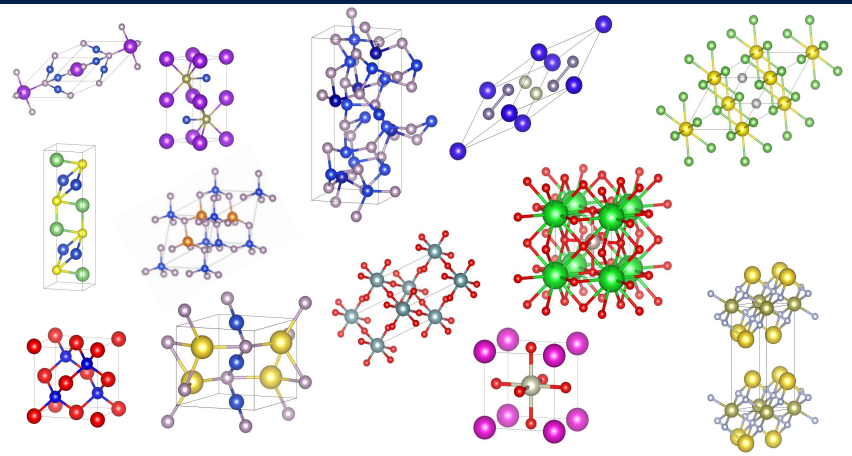
→ abiflows, atomate

...designed for our material-science applications !

What can we do with that ? A few examples of what has been done



Characterization of the electronic transport in materials

"An ab initio electronic transport database for inorganic materials", F. Ricci et al., Scientific data 4, 170085 (2017)

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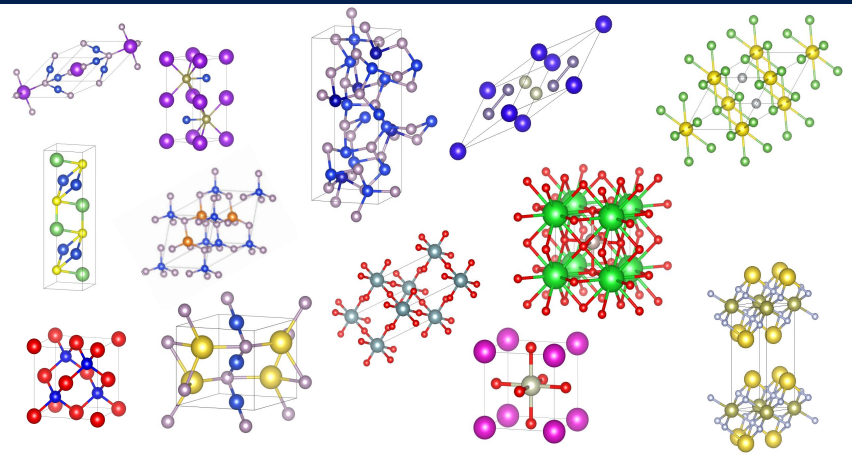

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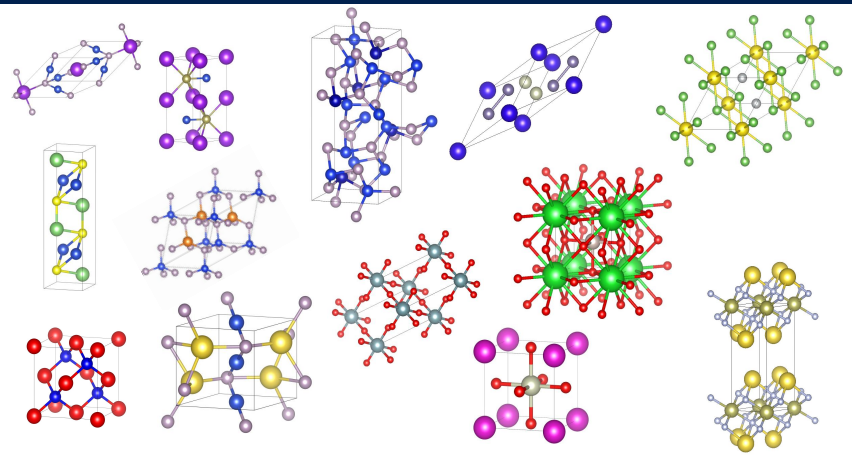

48000 materials

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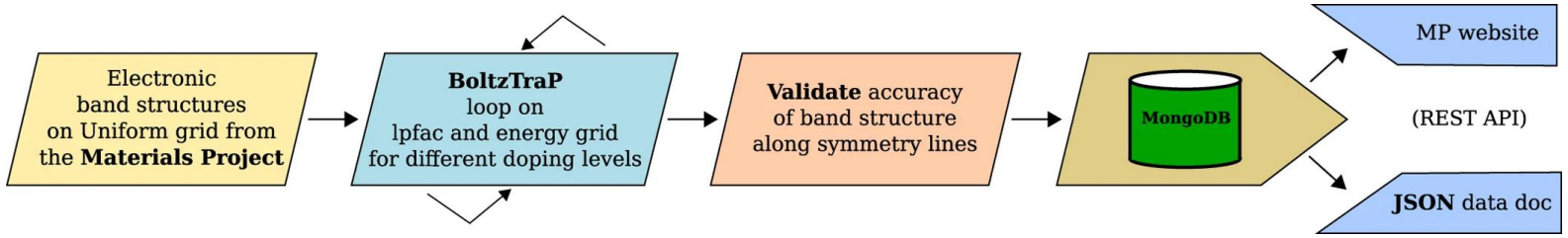

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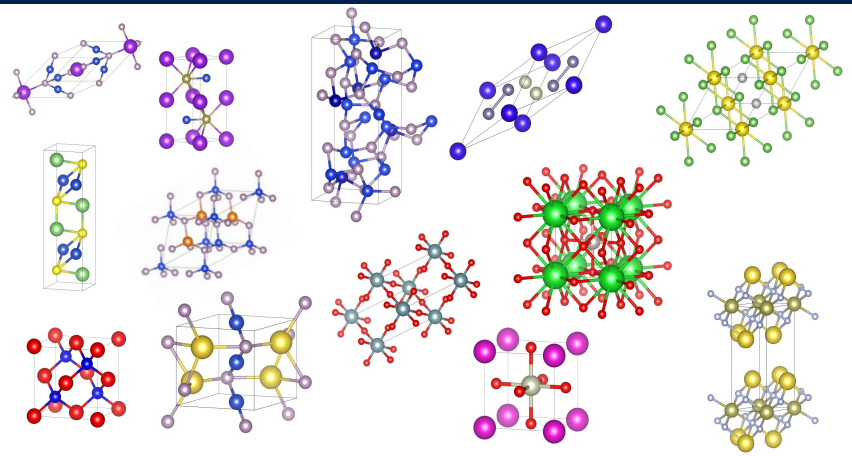

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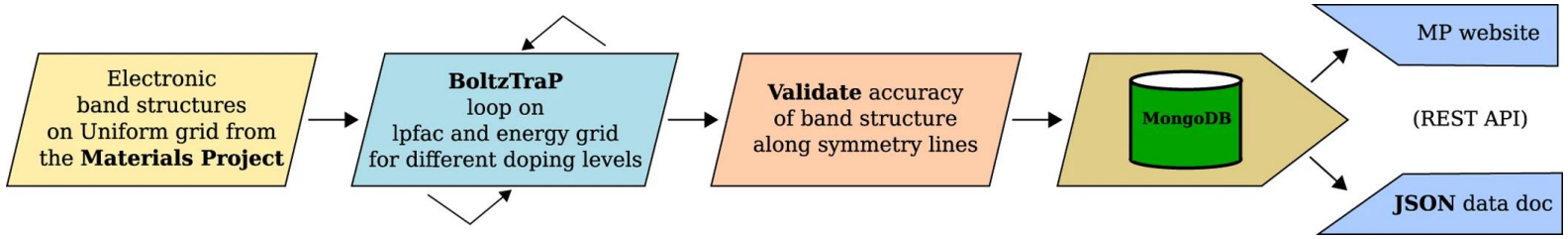

The results are now available in a database for all researchers !

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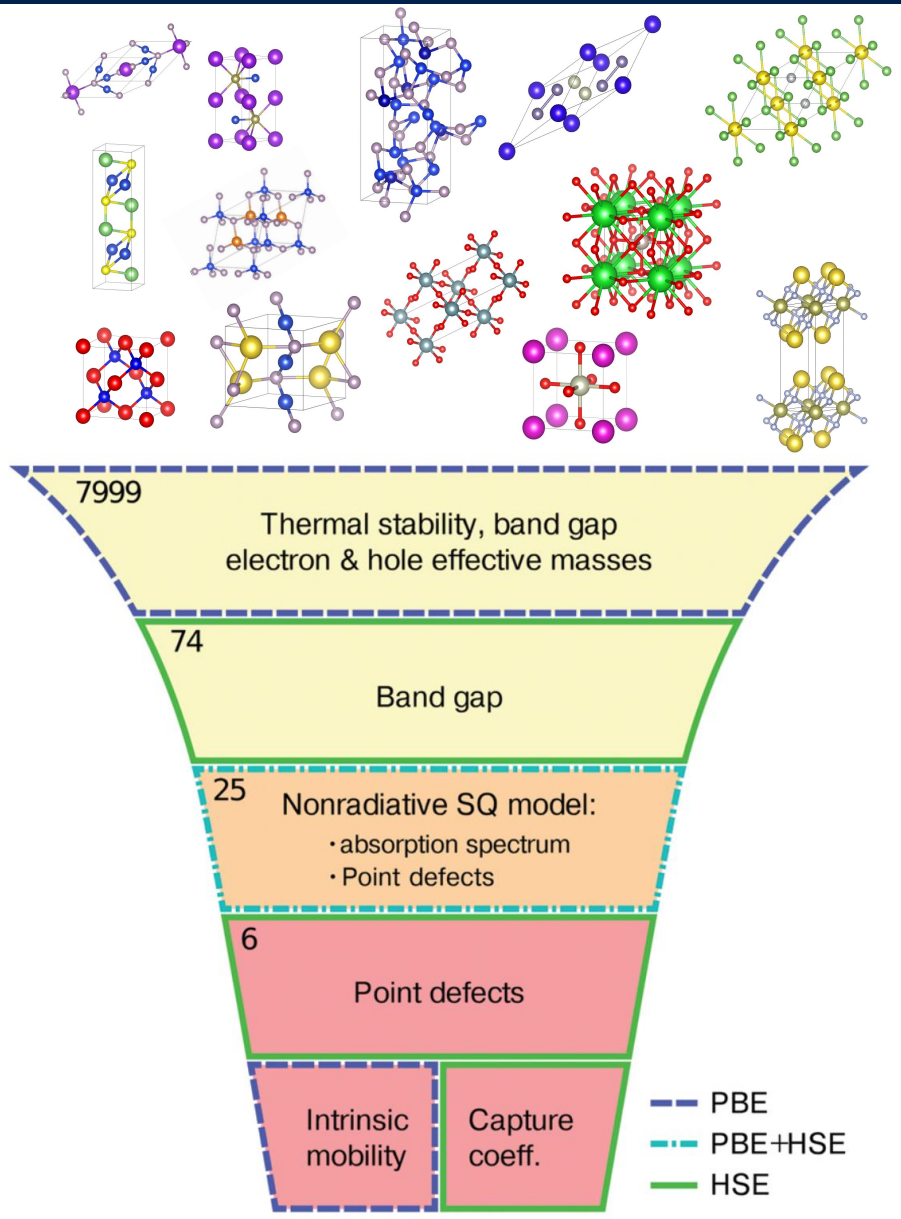

Looking for new materials for photovoltaics

"High-throughput computational search for high carrier lifetime, defect-tolerant solar absorbers", D. Dahliah et al., Energy & Environmental Science 14, 5057-5073 (2021)

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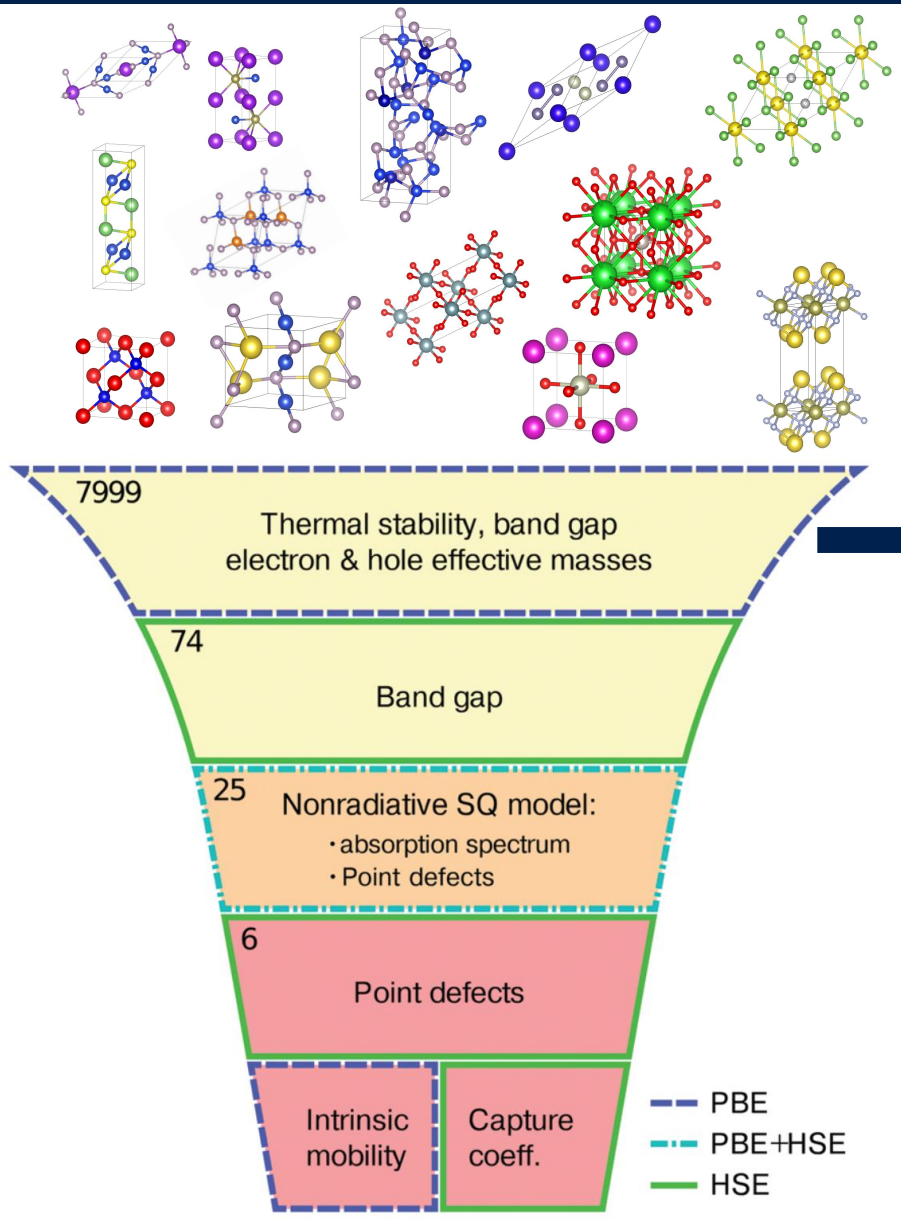

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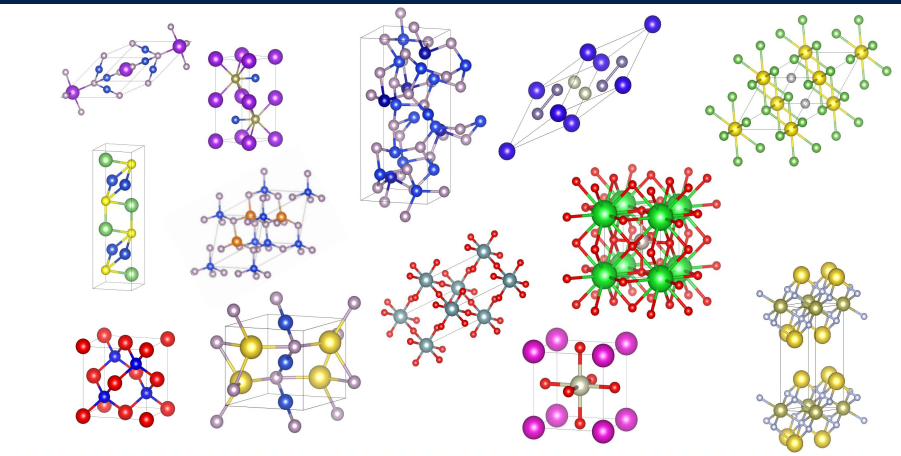

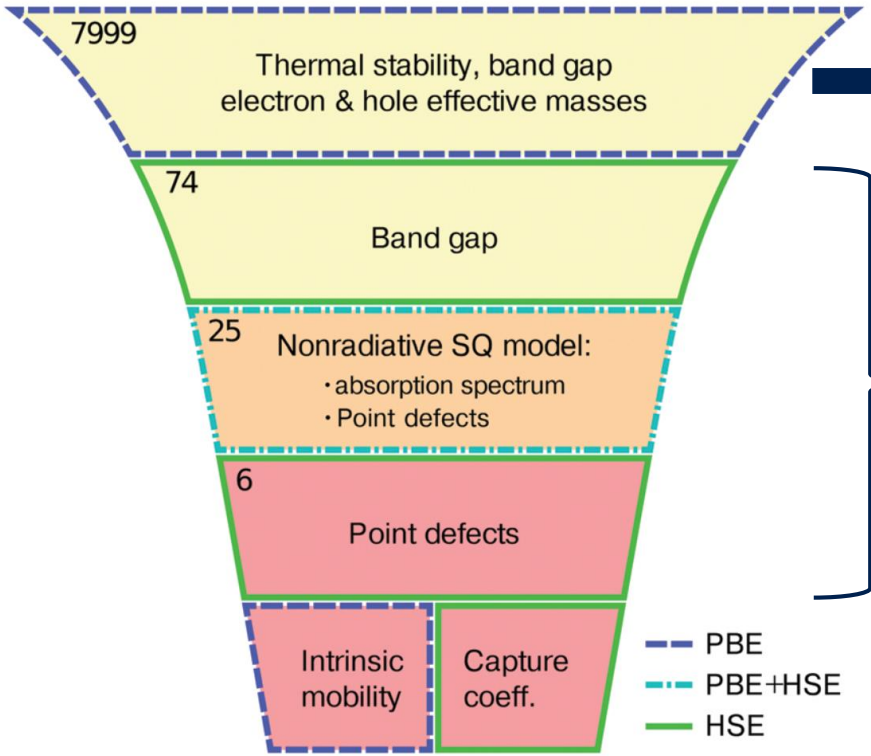

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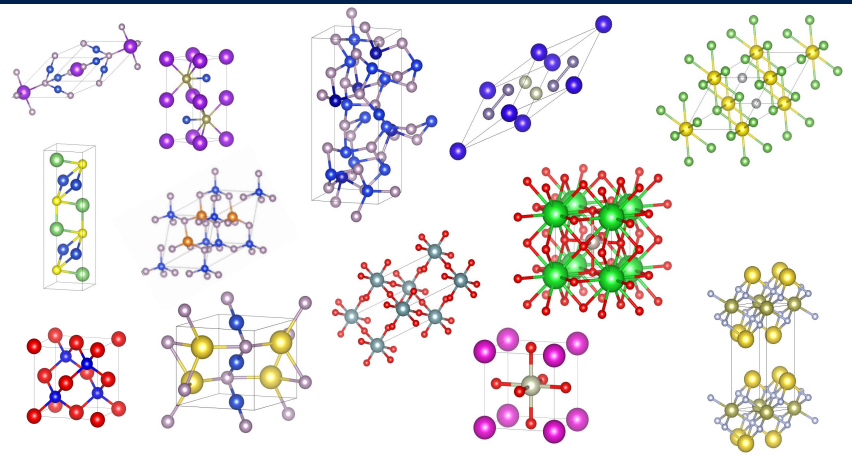
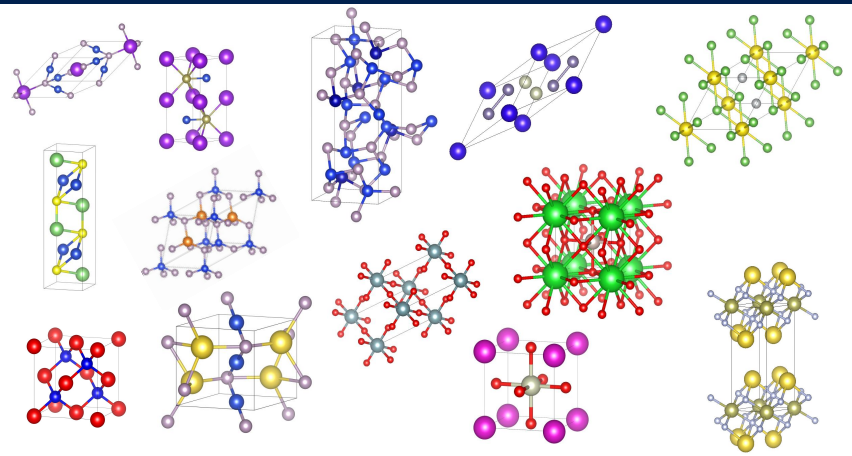


Computing the vibrational properties of materials (thermodynamics, transport,...)

"High-throughput density-functional perturbation theory phonons for inorganic materials", G. Petretto et al., Scientific Data 5, 180065 (2018)

What can we do with that ? A few examples of what has been done

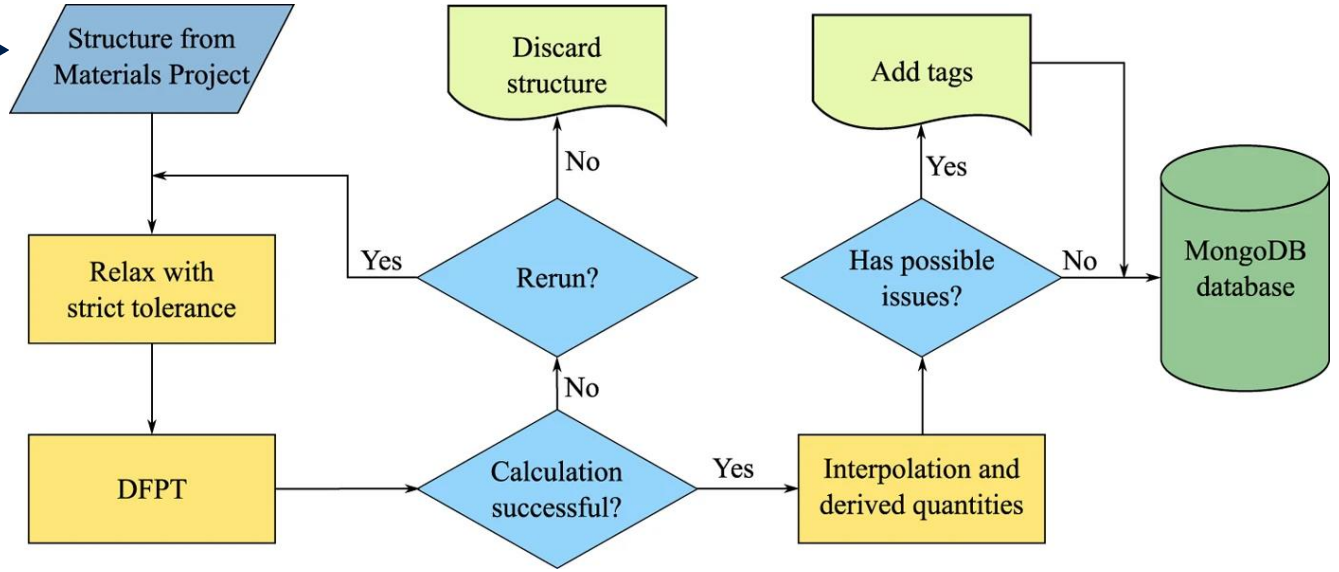


1521 materials

Computing the vibrational properties of materials (thermodynamics, transport,...)

abiflows

FireWorks



"High-throughput density-functional perturbation theory phonons for inorganic materials", G. Petretto et al., Scientific Data 5, 180065 (2018)

Take-home message

- Materials science sometimes require many computations
- FireWorks is a powerful tool to handle workflows
- It can be used in many applications : you should give it a try !

Thank you for your attention