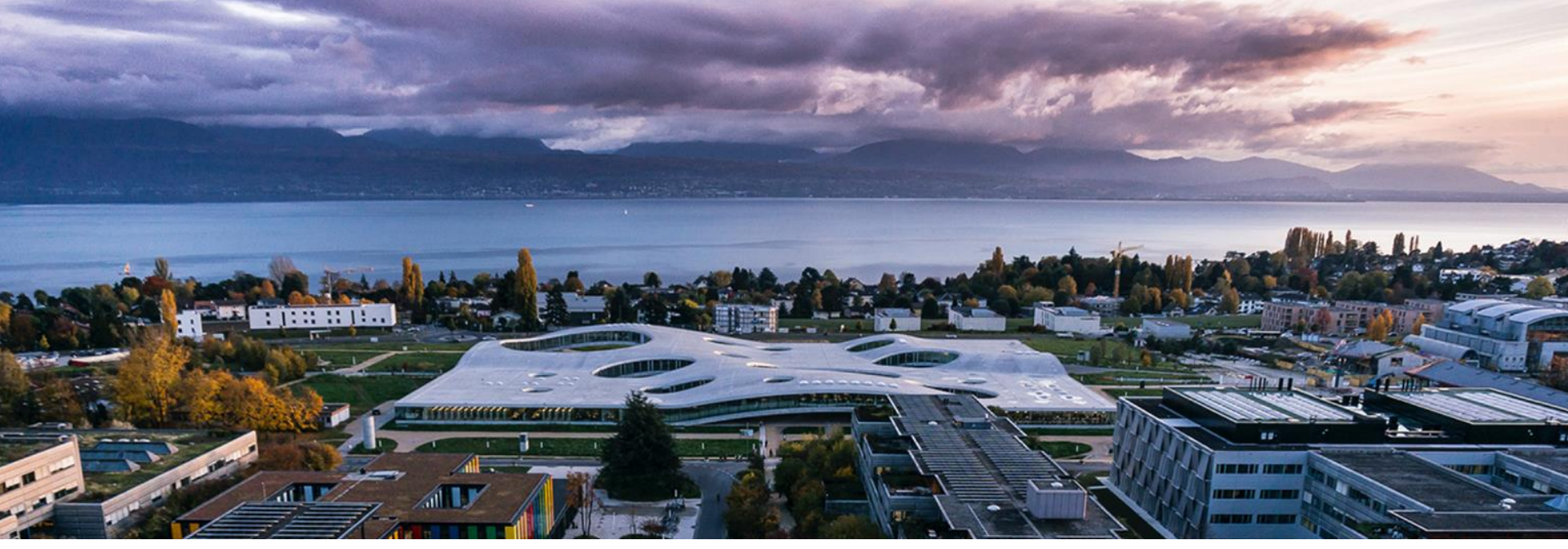

AiiDA & OPTIMADE

Casper Welzel Andersen

OPTIMADE
Open Databases Integration for Materials Design

MARVEL
MAX DRIVING THE EXASCALE TRANSITION
swissuniversities
FNSNF Swiss National Science Foundation
INTERSECT
MarketPlace
EPFL

OPTIMADE

Casper Welzel Andersen

A combined effort to create a common API (application programming interface) for materials structure databases.

Databases:

- Crystallography Open Database (COD)
- Materials Cloud
- The Materials Project
- The Novel Materials Discovery (NOMAD) Library
- Automatic - FLOW (AFLOW) for Materials Discovery
- The Open Quantum Materials Database (OQMD)
- Open Database of Xtals (ODBX)
- Joint Automated Repository for Various Integrated Simulations (JARVIS)
- ...

OPTIMADE

It is based on the JSON API v1.0.

Currently describes:

- Structures
- References

To come:

- Calculations

Can be used to access and report all `StructureData` Nodes in an AiiDA database through a REST API.

- Use **aiida-optimade** (found at https://github.com/aiidateam/aiida-optimade)
- To come: Native part of AiiDA as a DB importer.

OPTIMADE Client

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On Materials Cloud:

https://dev-tools.materialscloud.org/optimadeclient

On AiiDA lab:

Install the OPTIMADE Client app, see its entry in the AiiDA lab application registry here:

https://aiidalab.github.io/aiidalab-registry/apps/aiidalab-optimade.html

On your local machine:

- `git clone -b develop https://github.com/aiidalab/aiidalab-optimade`
- Install using `pip install -e aiidalab-optimade/`
- Run using `$ ./run.sh` from within the `aiidalab-optimade/` directory
- Go to http://localhost:8866

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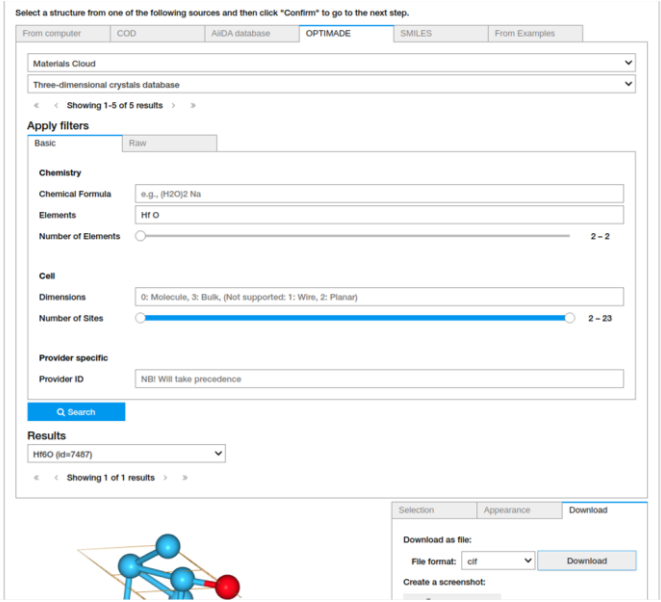
OPTIMADE Client

For AiiDA lab:

- Quickly retrieve structures from *any* OPTIMADE database for use in your AiiDA lab application/AiiDA workflow
- Integrate the client as a structure importer with any application

The Quantum ESPRESSO app:



A “SkyScanner”-like client also exists at

https://optimade.science

OPTIMADE Client

Casper Welzel Andersen

optimade_structure_7487.in - Notesblok

Filer Rediger Formater Vis Hjælp

```
&CONTROL
/
&SYSTEM
   ntyp            = 2
   nat             = 7
   ibrav           = 0
/
&ELECTRONS
/
&IONS
/
&CELL
/

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O 15.9994 O_dummy.UPF

K_POINTS gamma

CELL_PARAMETERS angstrom
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Hf 1.8562872480 3.2033683708 3.7927045754
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O 0.0000000000 0.0000000000 0.0000000000
```

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