

# Managing, simplifying and disseminating high-throughput computational materials science with AiiDA, AiiDA lab and the Materials Cloud Archive

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- > This is the second of a series of MaX webinars on the most recent developments of the MaX flagship codes
  - > first one on **Quantum ESPRESSO**
  - > next ones scheduled on **Yambo** and on **CP2K**, more to follow
- > <http://www.max-centre.eu/news/max-webinars>

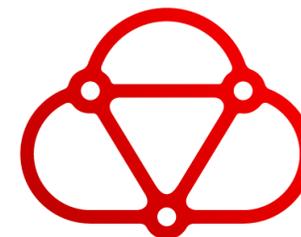
# Convergence of HPC, high-throughput and high-performance data analytics

- > Key focus in MaX: **Managing, simplifying and disseminating high-throughput computational materials science**
- > Deliverables to push for the convergence of
  - > high-performance computing (HPC)
  - > high-throughput computing (HTC)
  - > high-performance data analytics (HPDA)
- > Goals: push **open science, reproducible science**, and **FAIR sharing** of research data



<http://www.aiida.net>

The “**operating system**” to manage reproducibility, provenance-tracking, automation, and high-throughput



## MATERIALSCLOUD

<http://www.materialscloud.org>

The **web portal** for FAIR data dissemination, curated properties, online tools, cloud computing and educational material

# Today's presentations and presenters



The “**operating system**” to manage reproducibility, provenance-tracking, automation, and high-throughput



*“Introduction to AiiDA and use with QE-SIRIUS”*

by **Dr. Sebastiaan P. Huber** (EPFL)

(15:05-15:20 CEST)

# Today's presentations and presenters



Cloud simulations with AiiDA  
with powerful GUIs



**MATERIALS**CLOUD

# ARCHIVE

Long-term storage  
of data with DOIs



*"Turn-key solutions with AiiDA lab"*  
by **Dr. Aliaksandr Yakutovich** (EPFL)  
(15:20-15:35 CEST)

*"Depositing data on the Materials Cloud Archive"*

by **Dr. Valeria Granata** (EPFL)  
(15:35-15:50 CEST)



## Part of a larger community: **OPTIMADE**

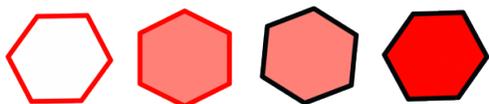
- > Part of the **OPTIMADE consortium**, together with 10+ other major crystal-structure databases
  - > Goal: provide standard API, allowing to run *the same query* against different databases
  - > <https://www.optimade.org>
- > If simulations are run with AiiDA, you can expose an OPTIMADE server
- > Data on the Materials Cloud can be accessed publicly via OPTIMADE queries

# The OPTIMADE client on the Materials Cloud (available soon)

The screenshot shows a web browser window with the URL `localhost:8866`. The page features the OPTIMADE logo (a network of colored nodes) and the text "OPTIMADE Open Databases Integration for Materials Design". Below the logo, it states "Currently valid OPTIMADE API version: v0.10.1" and provides a "Source code: GitHub" link. There are buttons for "Report a bug" and "Suggest a feature/change". A paragraph of text explains the client's purpose and provides links to the official web page and a GitHub issue. The interface includes sections for "FAQ" and "Log". A search area contains two dropdown menus for "Select a provider" and "No provider chosen", with a "Showing 0 of 0 results" indicator. A "Query" section has "Apply filters" and "Basic" tabs. The "Chemistry" section includes a "Chemical Formula" input field with the example "e.g., (H2O)2 Na" and an "Elements" selection grid with buttons for H, He, Li, Be, Na, Mg, B, C, N, O, F, Ne, Al, Si, P, S, Cl, and Ar. A "Results" section has a "Search for structures ..." dropdown and another "Showing 0 of 0 results" indicator.

# Other partner projects beside MaX

MARVEL



NATIONAL CENTRE OF COMPETENCE IN RESEARCH

<https://nccr-marvel.ch>



<https://www.the-marketplace-project.eu>



<http://intersect-project.eu>



Platform for Advanced Scientific Computing

<https://www.pasc-ch.org>

swissuniversities

<https://www.materialscloud.org/swissuniversities>



<https://www.ossicar.org>



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THE EXASCALE  
TRANSITION

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THANKS