MAX DRIVING THE EXASCALE TRANSITION

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

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Sebastiaan Huber, Aliaksandr Yakutovich, Valeria Granata (Speakers), EPFL

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MaX "*Materials Design at the Exascale*", has received funding from the European Union's Horizon 2020 project call H2020-INFRAEDI-2018-1, grant agreement 824143

MaX webinars

- 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**

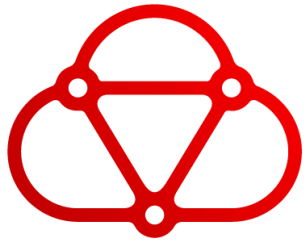
- Deliverables to push for the convergence of
  - high-performance computing (HPC)
  - high-throughput computing (HTC)
  - high-performance data analytics (HPDA)

- Goals: push **open science**, **reproducible science**, and **FAIR sharing** of research data

Tools of choice: AiiDA and Materials Cloud

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

AiiDA

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

AiiDAlab

Cloud simulations with AiiDA with powerful GUIs

MATERIALSCLOUD

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)

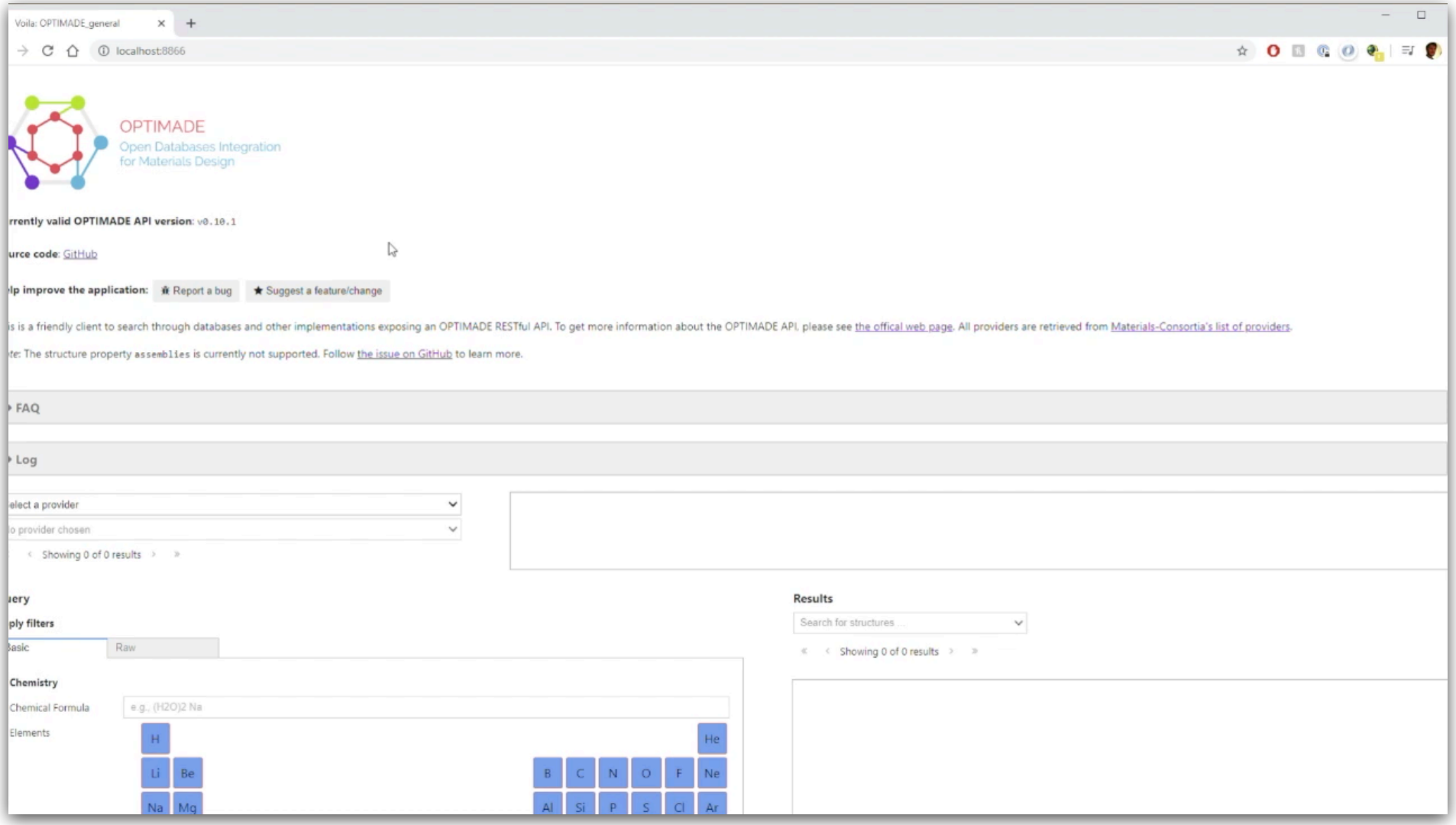
(15:35-15:50 CEST)

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)



Client developed by Casper W. Andersen, EPFL

Other partner projects beside MaX

MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

https://nccr-marvel.ch

MarketPlace

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

INTERSECT

http://intersect-project.eu

pasc
Platform for Advanced Scientific Computing

https://www.pasc-ch.org

swissuniversities

https://www.materialscloud.org/swissuniversities

OSSCAR

https://www.osscar.org

DRIVING
THE EXASCALE
TRANSITION

THANKS

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