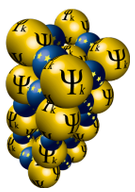
MATERIALSCLOUD

The Materials Cloud

Writing reproducible workflows using AiiDA

May 21st-24th, 2019, Lausanne



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MAX DRIVING THE EXASCALE TRANSITION

INTERSECT

swissuniversities

EPFL

The OSP - Vision

Computational Materials Science Challenges

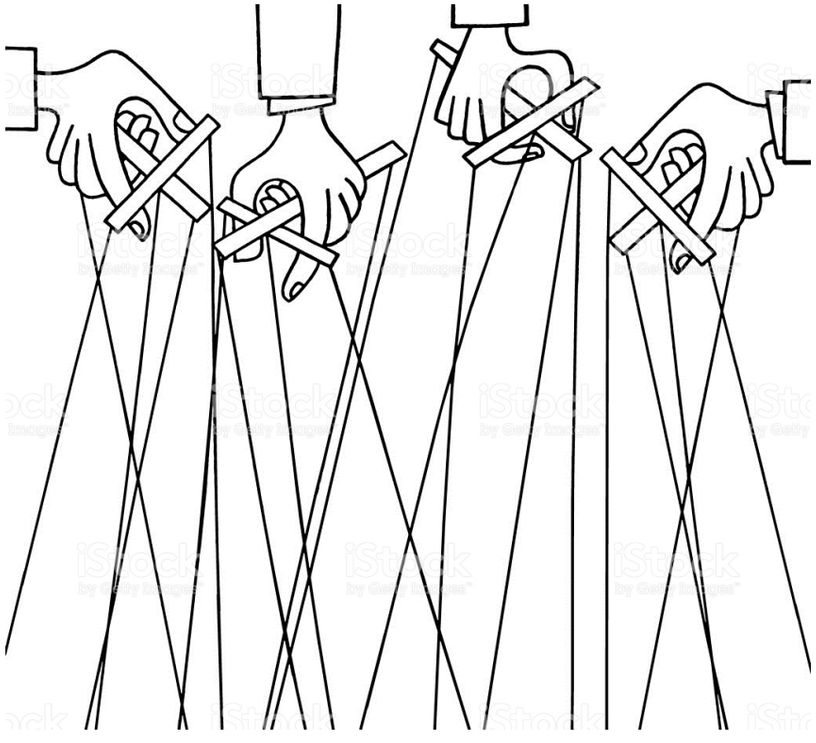
High-Throughput

Reproducibility

Open Data

Knowledge Transfer

- Organize large numbers of calculations
- Deal with corner cases (theory, code, infrastructure)
- Many strings to pull



Source: istockphoto.com

AiiDA

The OSP - Vision

Computational Materials Science Challenges

High-Throughput

Reproducibility

Open Data

Knowledge Transfer

- Keep track of what you calculate
- Keep track of how you did it
- Within a research group:
  Can Alice reproduce what Bob computed 1 year ago?

AiiDA

Source: academiccoachingandwriting.org

The OSP - Vision

Computational Materials Science Challenges

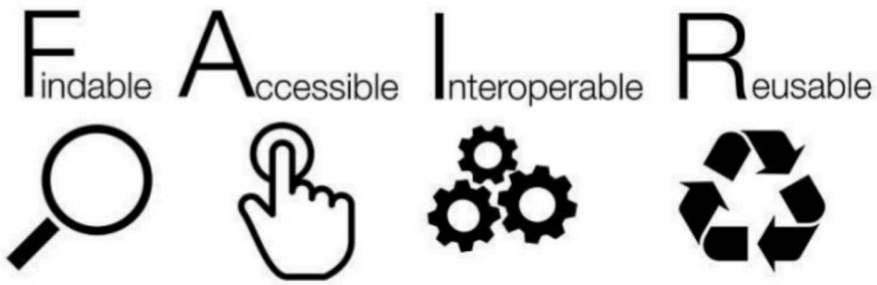
High-Throughput

Reproducibility

Open Data

Knowledge Transfer

- Open Data
  - ~~Supporting Information~~
  - ~~Just upload everything~~
  - FAIR data
- Making data FAIR is hard, can we make it easier?



Source: Prof. Michel Dumontier

AiiDA + MATERIALS CLOUD

The OSP - Vision

Computational Materials Science Challenges

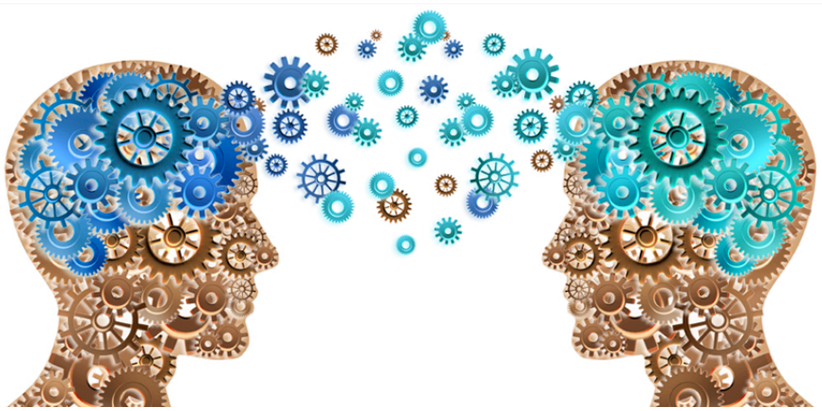
High-Throughput

Reproducibility

Open Data

Knowledge Transfer

- Share a workflow for your code with a collaborator or company
- Share the environment needed to run the workflow
- Reduce email traffic by sharing access to live dashboards with simulation results
- ...



Source: quote.ucsd.edu

AiiDAlab

Materials Cloud

- **AiiDA** is the 'engine', like **Git -** used in production since 2015
- **Materials Cloud** is the dissemination platform (like **GitHub**) **and more** (cloud computing and data generation platform) - online since Dec 2017

Materials Cloud

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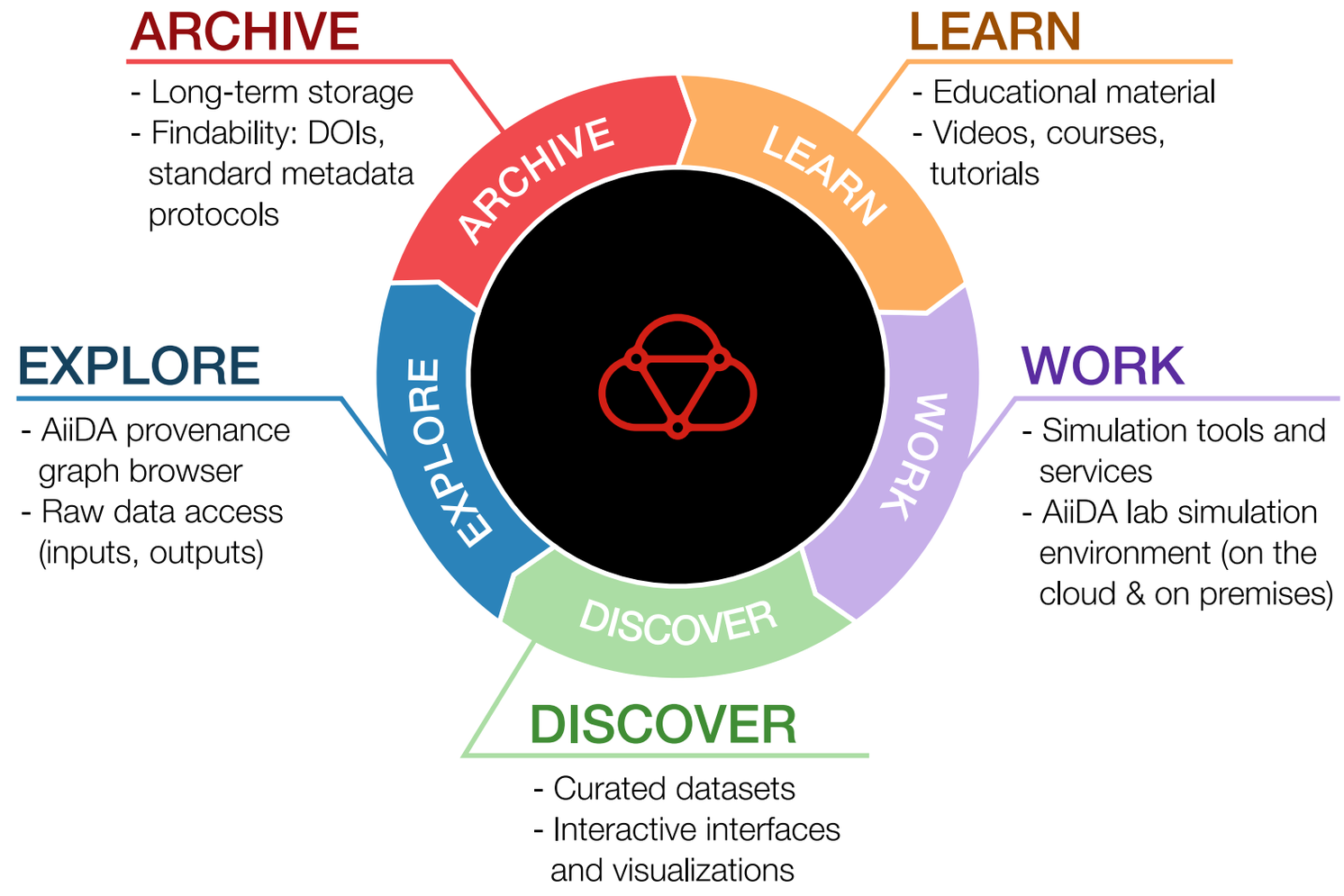

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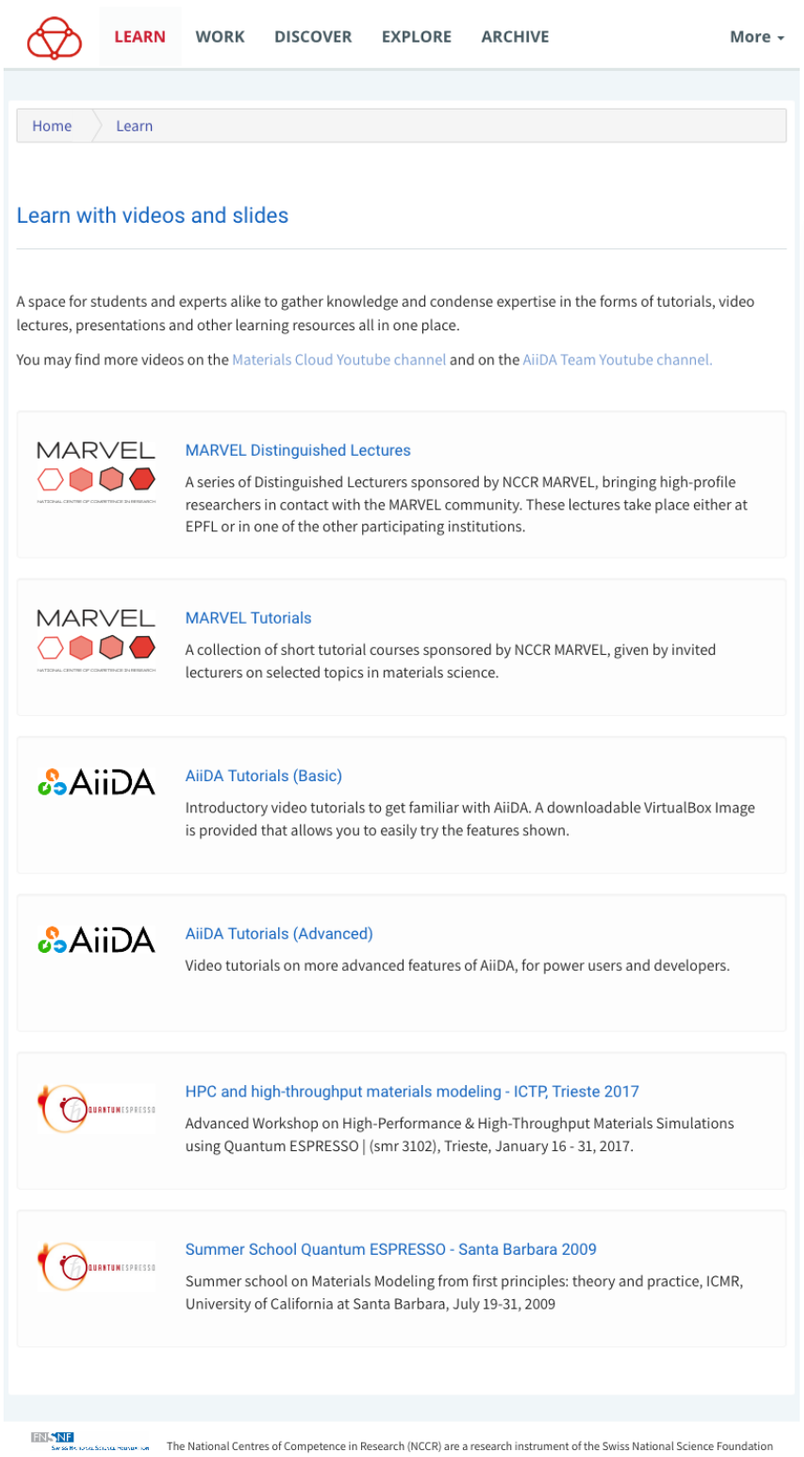
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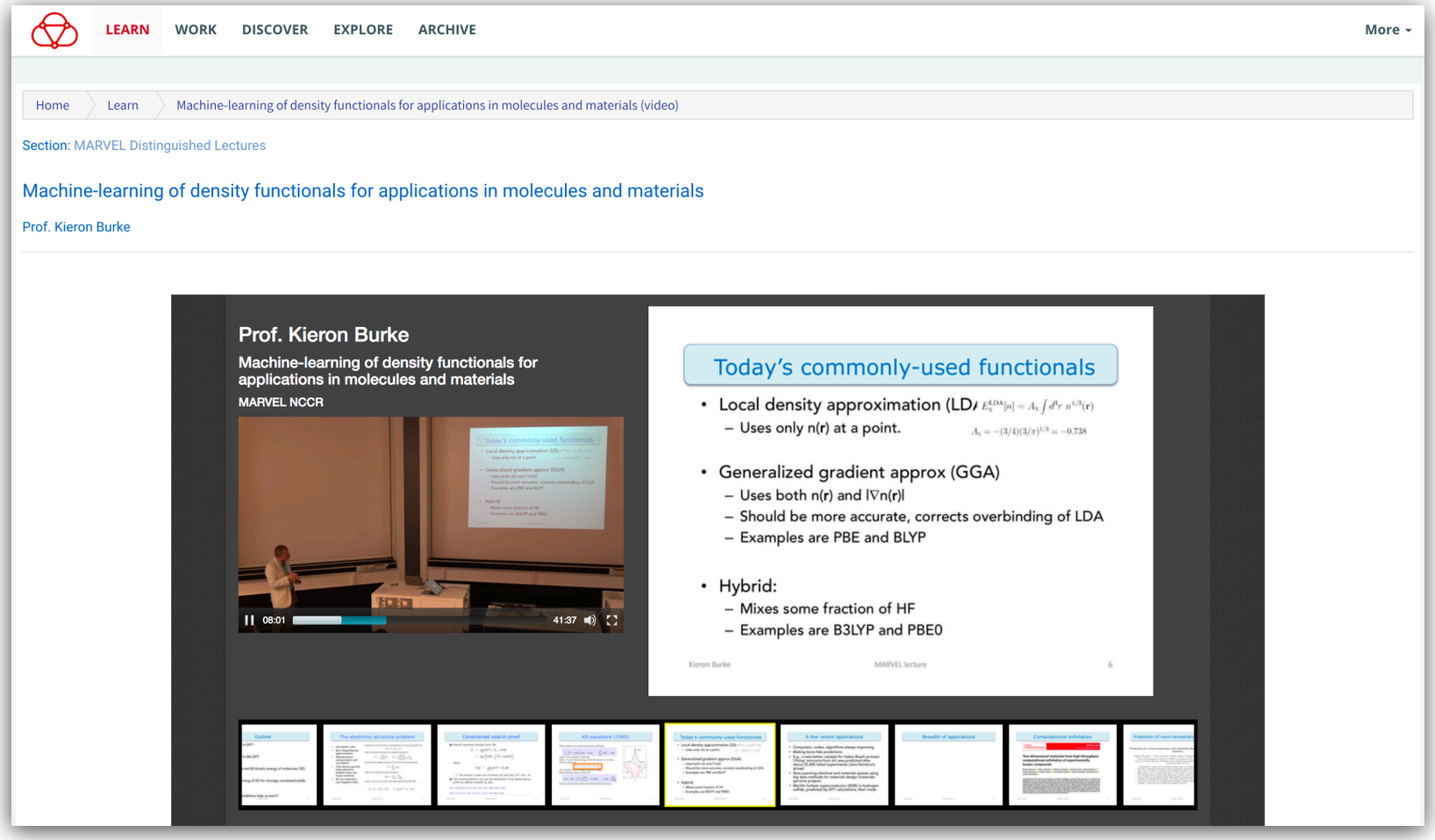
A space for students and experts alike to gather knowledge and condense expertise in the forms of tutorials, video lectures, presentations and other learning resources all in one place.
You may find more videos on the Materials Cloud Youtube channel and on the AiiDA Team Youtube channel.
MARVEL Distinguished Lectures
A series of Distinguished Lecturers sponsored by NCCR MARVEL, bringing high-profile researchers in contact with the MARVEL community. These lectures take place either at EPFL or in one of the other participating institutions.
MARVEL Tutorials
A collection of short tutorial courses sponsored by NCCR MARVEL, given by invited lecturers on selected topics in materials science.
AiiDA Tutorials (Basic)
Introductory video tutorials to get familiar with AiiDA. A downloadable VirtualBox Image is provided that allows you to easily try the features shown.
AiiDA Tutorials (Advanced)
Video tutorials on more advanced features of AiiDA, for power users and developers.
HPC and high-throughput materials modeling - ICTP, Trieste 2017
Advanced Workshop on High-Performance & High-Throughput Materials Simulations using Quantum ESPRESSO | (smr 3102), Trieste, January 16 - 31, 2017.
Summer School Quantum ESPRESSO - Santa Barbara 2009
Summer school on Materials Modeling from first principles: theory and practice, ICMR, University of California at Santa Barbara, July 19-31, 2009
The National Centres of Competence in Research (NCCR) are a research instrument of the Swiss National Science Foundation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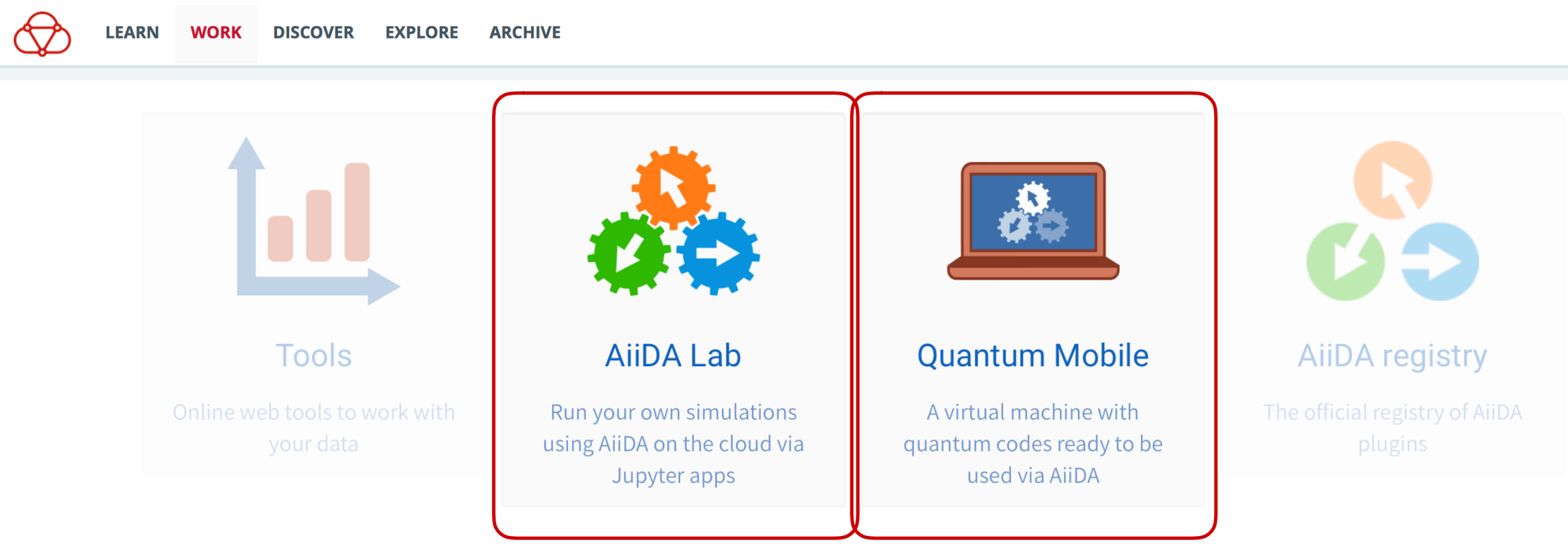
Machine-learning of density functionals for applications in molecules and materials (video)
Section: MARVEL Distinguished Lectures
Machine-learning of density functionals for applications in molecules and materials
Prof. Kieron Burke
Prof. Kieron Burke
Machine-learning of density functionals for applications in molecules and materials
MARVEL NCCR
08:01
41:37
Today's commonly-used functionals
Local density approximation (LDA)
Uses only n(r) at a point.
Generalized gradient approx (GGA)
Uses both n(r) and |∇n(r)|
Should be more accurate, corrects overbinding of LDA
Examples are PBE and BLYP
Hybrid:
Mixes some fraction of HF
Examples are B3LYP and PBE0
Kieron Burke
MARVEL lecture
6

Data generation: Materials Cloud Work



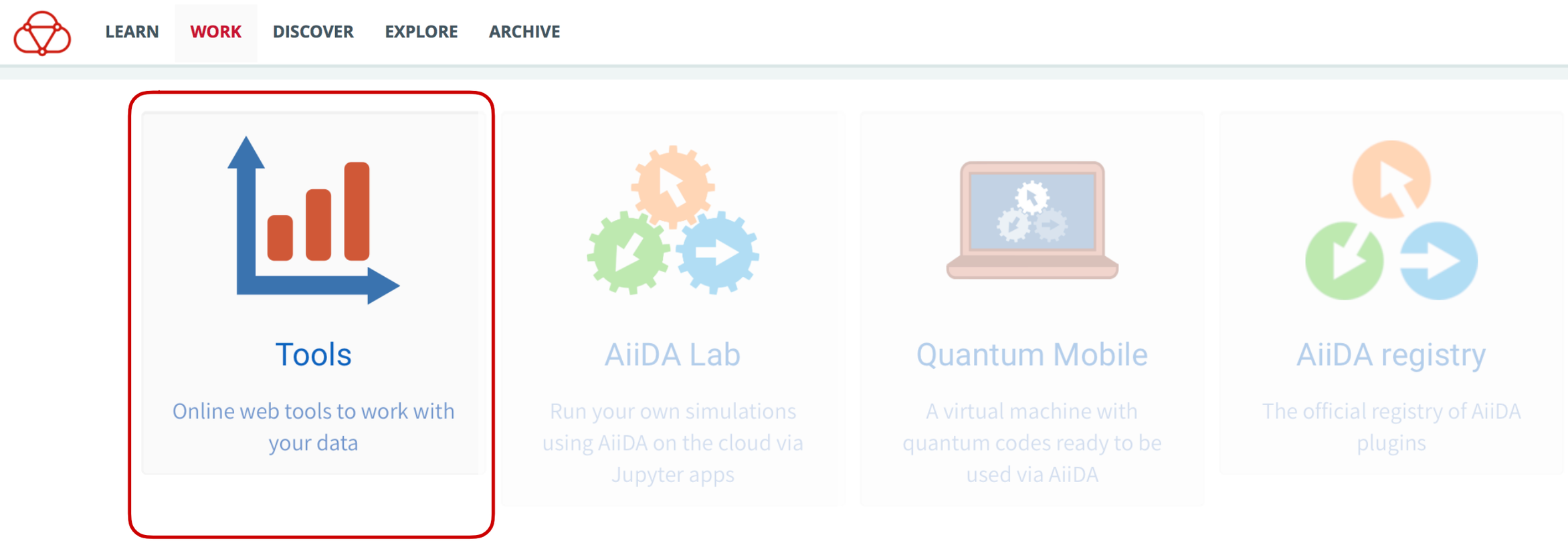
AiiDA Lab

- Comes with a preconfigured AiiDA setup, **ideal interface for turn-key workflows**
- Custom **AppMode** extension to make notebooks look&feel like real web apps knowing only python
- Using JupyterHub + DockerSpawner

Quantum Mobile

- **Downloadable VM** with preinstalled **AiiDA and codes** like QE, Yambo, Fleur, Siesta, CP2K, …
- Includes **same AiiDA Lab apps environment** as on Materials Cloud
- Ideal for **education**

Data generation: Materials Cloud Work



Tools

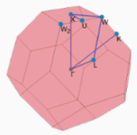
- Simple web-based applications that allow to run simulations within a few seconds (~<10-60 sec)
- Useful to provide visualisation

Data generation: Materials Cloud Work

Tools

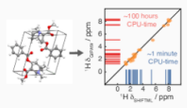
Add new tool

Computational tools offered as a service: no download, no installation, but click-and-run.



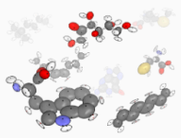
SeeK-path: the k-path finder and visualizer

Authors: Yoyo Hinuma, Giovanni Pizzi, Yu Kumagai, Fumiyasu Oba, Isao Tanaka
Description: A k-path finder that provides band paths compatible with space group symmetry, and an interactive 3D visualizer.



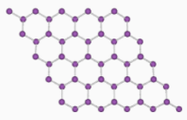
ShiftML: chemical shifts in molecular crystals by machine learning

Authors: Federico M. Paruzzo, Albert Hofstetter, Félix Musil, De Sandip, Michele Ceriotti, and Lyndon Emsley
Description: A machine learning model to predict the isotropic chemical shielding of molecular crystals containing H, C, N and O, and an interactive 3D visualiser.



AlphaML: machine learning of molecular polarizabilities

Authors: David M. Wilkins, Andrea Grisafi, Yang Yang, Ka Un Lao, Robert A. DiStasio Jr. and Michele Ceriotti
Description: A machine learning framework for the prediction of molecular polarizabilities based on comparisons of local environments.



Interactive phonon visualizer

Authors: Snehal Kumbhar, Giovanni Pizzi, Thibault Sohier, Henrique Miranda
Description: A tool for the interactive visualization and inspection of lattice vibrations.

SyCoFinder

Synthesis condition finder

Authors: Seyed Mohamad Moosavi, Leopold Talirz
Description: A tool for optimizing the experimental synthesis conditions for metal-organic frameworks using machine learning and genetic algorithms.

Data generation: Materials Cloud Work

Tools

Add new tool

SeeK-path: the *k*-path finder and visualizer

▸ What SeeK-path does

▸ SeeK-path definitions and advantages

Upload your structure

Upload a crystal structure: Choose File no file selected

Select here the file format: Quantum ESPRESSO input [parser: qe-tools]

By continuing, you agree with the terms of use of this service.

Calculate my structure

Otherwise, pick an example

Select here an extended Bravais Symbol: aP2 [with inversion]

A simple explanation of the extended Bravais symbols.

Calculate this example

How to cite

If you use this tool, please cite the following work:

- Y. Hinuma, G. Pizzi, Y. Kumagai, F. Oba, I. Tanaka, Band structure diagram paths based on crystallography, Comp. Mat. Sci. 128, 140 (2017). DOI: 10.1016/j.commatsci.2016.10.015 (the "HPKOT" paper; arXiv version: arXiv:1602.06402).
- You should also cite Spglib that is an essential library used in the implementation.
- The input parsers use a number of libraries (see name in the dropdown list) from ASE, qe-tools or pymatgen.

Note: if you want to use the code on your computer, you can download the SeeK-path python library from the SeeK-path GitHub repository.

SyCoFinder

using machine learning and genetic algorithms.

MAX DRIVING THE EXASCALE TRANSITION

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EPFL

Data generation: Materials Cloud Work

Tools

Add new tool

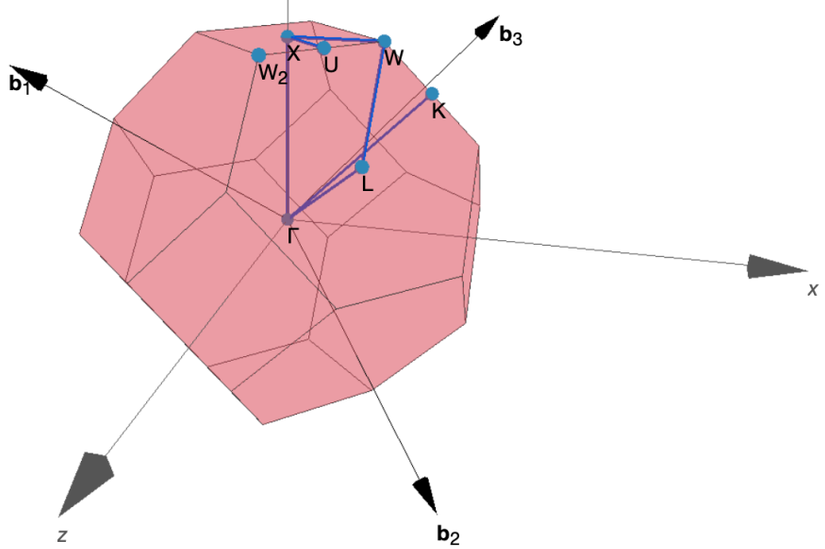
SeeK-path: the *k*-path finder and visualizer

▸ Show parsed input coordinates (please double-check here if the parser worked properly)

Jump directly to downloadable coordinates

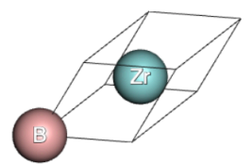
Brillouin zone (go to coordinates)

Drag to rotate, scroll to zoom, double-click to enable/disable interaction



Primitive structure (go to coordinates)

Drag to rotate, scroll to zoom, double-click to enable/disable interaction



Note: if you want to use the code on your computer, you can download the SeeK-path python library from the SeeK-path GitHub repository.

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Reciprocal space and Brillouin-zone information

Reciprocal cell vectors (1/Å)

b	x	y	z
b_1	-1.2789831717	1.2789831717	1.2789831717
b_2	1.2789831717	-1.2789831717	1.2789831717
b_3	1.2789831717	1.2789831717	-1.2789831717

High-symmetry points (scaled units)

Label	k_1	k_2	k_3
Γ	0.0000000000	0.0000000000	0.0000000000
K	0.3750000000	0.3750000000	0.7500000000
L	0.5000000000	0.5000000000	0.5000000000
U	0.6250000000	0.2500000000	0.6250000000
W	0.5000000000	0.2500000000	0.7500000000
W_2	0.7500000000	0.2500000000	0.5000000000
X	0.5000000000	0.0000000000	0.5000000000

High-symmetry points (1/Å)

Label	k_x	k_y	k_z
Γ	0.0000000000	0.0000000000	0.0000000000
K	0.9592373788	0.9592373788	0.0000000000
L	0.6394915858	0.6394915858	0.6394915858
U	0.3197457929	1.2789831717	0.3197457929
W	0.6394915858	1.2789831717	0.0000000000
W_2	0.0000000000	1.2789831717	0.6394915858
X	0.0000000000	1.2789831717	0.0000000000

Suggested path

Γ—X—U|K—Γ—L—W—X

Structure information (primitive cell)

Crystal structure information

Bravais lattice type: cF

Extended Bravais lattice symbol: cF2 (with inversion symmetry)

Spacegroup: Fm-3m (number 225)

Primitive cell vectors (Å)

v	x	y	z
v_1	0.0000000000	2.4563205546	2.4563205546
v_2	2.4563205546	0.0000000000	2.4563205546
v_3	2.4563205546	2.4563205546	0.0000000000

Atom coordinates (scaled)

Element	r_1	r_2	r_3
B	0.0000000000	0.0000000000	0.0000000000
Zr	-0.5000000000	0.5000000000	0.5000000000

Atom coordinates (Cartesian, Å)

Element	x	y	z
B	0.0000000000	0.0000000000	0.0000000000
Zr	2.4563205546	0.0000000000	0.0000000000

SyCoFinder

using machine learning and genetic algorithms.

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Data generation: Materials Cloud Work

Tools

Add new tool

Computational tools offered as a service: no download, no installation, but click-and-run.

Phonon dispersion: Bi_2

Drag to rotate, scroll to zoom

Phonon band structure (select phonon)

Settings

Repetitions: 5 5 1 update

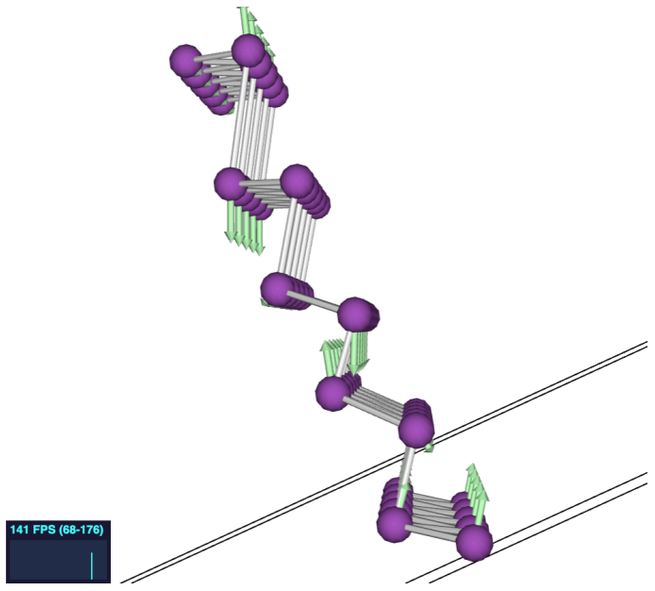
Camera: x y z

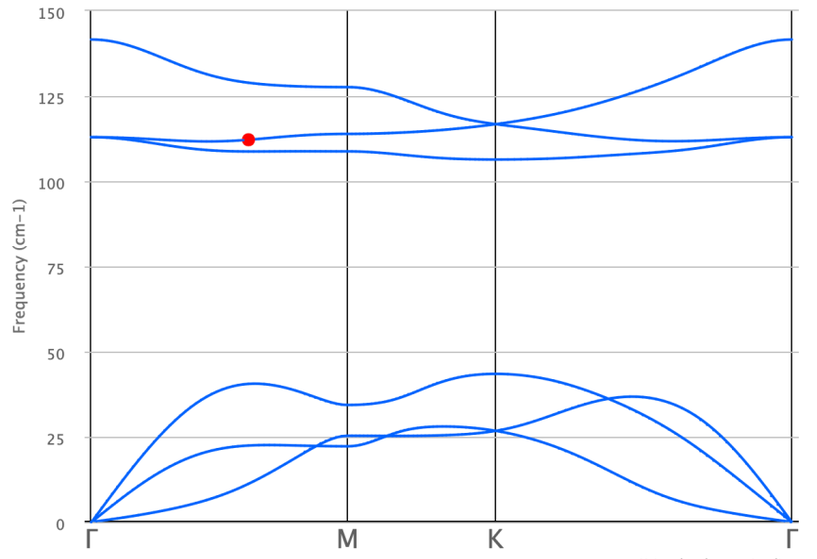
Cell: on

Amplitude: 0.65

Vectors: on

Speed: pause





Lattice parameters (Ångström):

4.297	0.000	0.000
-2.149	3.722	0.000
0.000	0.000	21.67

Atomic positions (reduced):

Bi	0.6667	0.3333	0.4597
Bi	0.3333	0.6667	0.5403

SyCoFinder

Authors: Seyed Mohamad Moosavi, Leopold Talirz
Description: A tool for optimizing the experimental synthesis conditions for metal-organic frameworks using machine learning and genetic algorithms.

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Open and FAIR data sharing: **Archive, Discover, Explore**

materialscloud:2017.0008

SCIENTIFIC DATA

re3data.org REGISTRY OF RESEARCH DATA REPOSITORIES http://doi.org/10.17616/R3ZJ5W Materials Cloud

FAIRsharing.org standards, databases, policies

Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds

Authors: Nicolas Mounet[1*], Marco Gibertini[1], Philippe Schwaller[1], Davide Campi[1], Andrius Merkys[1,2], Antimo Marrazzo[1], Thibault Sohier[1], Ivano E. Castelli[1], Andrea Cepellotti[1], Giovanni Pizzi[1], Nicola Marzari[1*]

1 Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

2 Vilnius University Institute of Biotechnology, Sauletekio al. 7, LT-10257 Vilnius, Lithuania

* Corresponding authors emails: nicolas.mounet@epfl.ch, nicola.marzari@epfl.ch

DOI 10.24435/materialscloud:2017.0008/v2 (version v2, submitted on 21 March 2018)

How to cite this entry

Nicolas Mounet, Marco Gibertini, Philippe Schwaller, Davide Campi, Andrius Merkys, Antimo Marrazzo, Thibault Sohier, Ivano E. Castelli, Andrea Cepellotti, Giovanni Pizzi, Nicola Marzari, *Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds*, Materials Cloud Archive (2018), doi: 10.24435/materialscloud:2017.0008/v2.

Description

Two-dimensional (2D) materials have emerged as promising candidates for next-generation electronic and optoelectronic applications. Yet, only a few dozens of 2D materials have been successfully synthesized or exfoliated. Here, we search for novel 2D materials that can be easily exfoliated from their parent compounds. Starting from 108423 unique, experimentally known three-dimensional compounds we identify a subset of 5619 that appear layered according to robust geometric and bonding criteria. High-throughput calculations using van-der-Waals density-functional theory, validated against experimental structural data and calculated random-phase-approximation binding energies, allow to identify 1825 compounds that are either easily or potentially exfoliable. In particular, the subset of 1036 easily exfoliable cases provides novel structural prototypes and simple ternary compounds as well as a large portfolio of materials to search from for optimal properties. For a subset of 258 compounds we explore vibrational, electronic, magnetic, and topological properties, identifying 56 ferromagnetic and antiferromagnetic systems, including half-metals and half-semiconductors. This archive entry contains the database of 2D materials (structural parameters, band structures, binding energies, etc.) together with the provenance of all data and calculations as stored by AiiDA.

Materials Cloud sections using this data

Select 2d materials via interactive periodic table and view their properties (with links to provenance)

Explore interface providing access to the full database

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Open and FAIR data sharing: **Archive, Discover, Explore**

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Direct links to Discover & Explore

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FAIRsharing.org
re3data.org

+

Recommended data repository by Nature's journal Scientific Data

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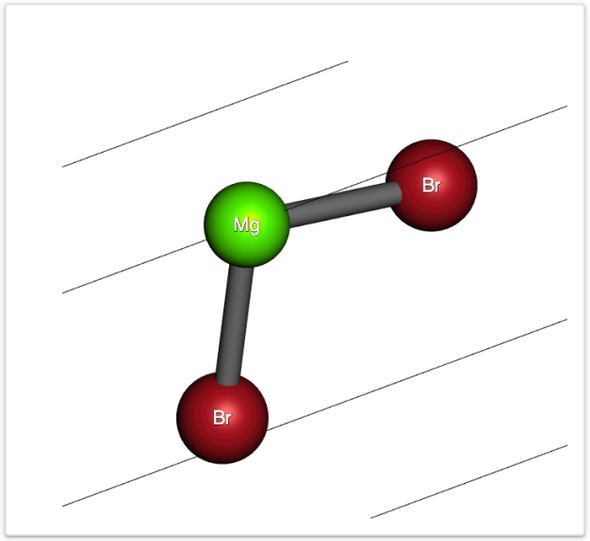
DISCOVER (CURATED DATA) & EXPLORE (RAW DATA)

DISCOVER

Compound: $MgBr_2$



Info and properties

See definitions...

Formula: $MgBr_2$
Spacegroup: P-3m1
Pointgroup: -3m
Prototype: CdI2
Band gap [eV]: 4.8

Magnetic properties:

- Magnetic State: non-magnetic
- Tot. Magnetization [μB/cell]: -
- Abs. Magnetization [μB/cell]: -

Binding Energies:

- DF2-C09 Binding energy [meV/Å^2]: 10.2
  (From parent COD 9009107)
- rVV10 Binding energy [meV/Å^2]: 15.3
  (From parent COD 9009107)

Delta in interlayer distance (vdW vs revPBE):

- Δ_{DF2} [%]: 17.1 (From parent COD 9009107)
- Δ_{rVV10} [%]: 18.3 (From parent COD 9009107)

Band structure

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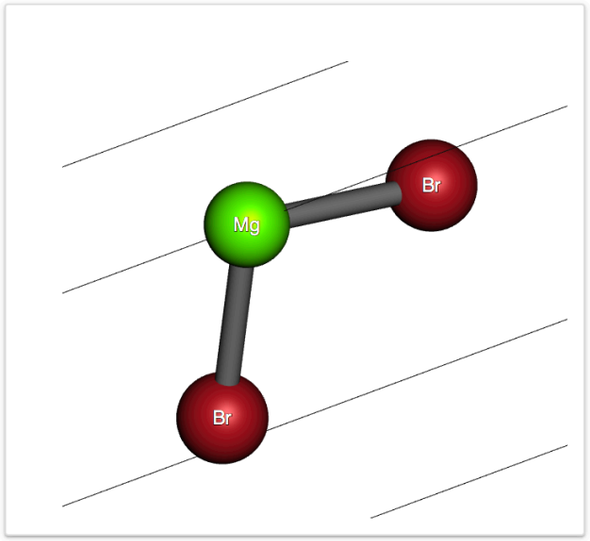
DISCOVER (CURATED DATA) & EXPLORE (RAW DATA)

DISCOVER

Compound: $MgBr_2$



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- DF2-C09 Binding energy [meV/Å^2]: 10.2 (From parent COD 9009107)
- rVV10 Binding energy [meV/Å^2]: 15.3 (From parent COD 9009107)

Delta in interlayer distance (vdW vs revPBE):

- Δ_{DF2} [%]: 17.1 (From parent COD 9009107)
- Δ_{rVV10} [%]: 18.3 (From parent COD 9009107)

Band structure

UUID links to jump to the provenance graph in the EXPLORE section

DRIVING THE EXASCALE TRANSITION

MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Materials Cloud

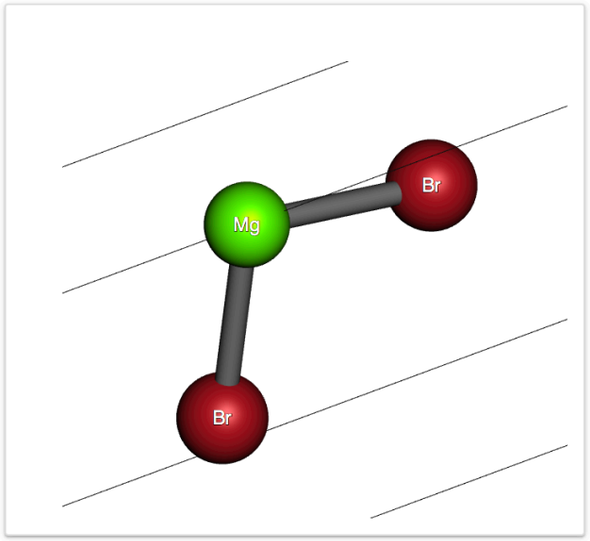
swissuniversities

EPFL

DISCOVER (CURATED DATA) & EXPLORE (RAW DATA)

DISCOVER

Compound: $MgBr_2$



Info and properties

See definitions...

Formula: $MgBr_2$
Spacegroup: P-3m1
Pointgroup: -3m
Prototype: CdI2
Band gap [eV]: 4.8

Magnetic properties:
- Magnetic State: non-magnetic
- Tot. Magnetization [μB/cell]: -
- Abs. Magnetization [μB/cell]: -

Binding Energies:
- DF2-C09 Binding energy [meV/Å^2]:
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- rVV10 Binding energy [meV/Å^2]: 15
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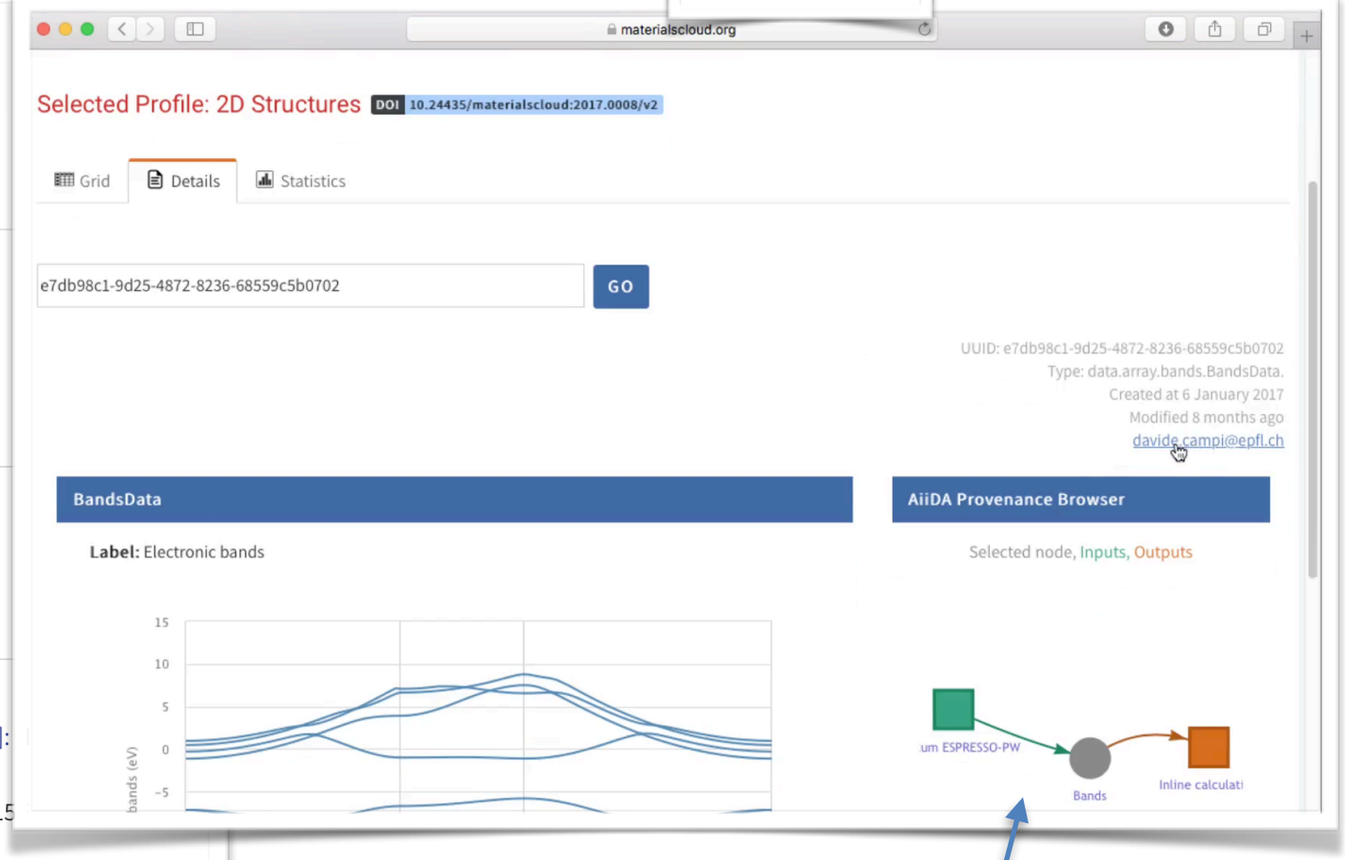

UUID links to jump to the provenance graph in the EXPLORE section

Browse the full AiiDA provenance graph (inputs, outputs, …) at any level

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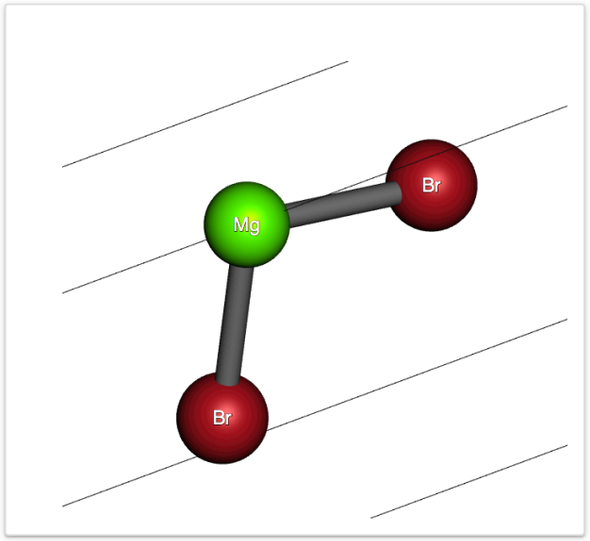

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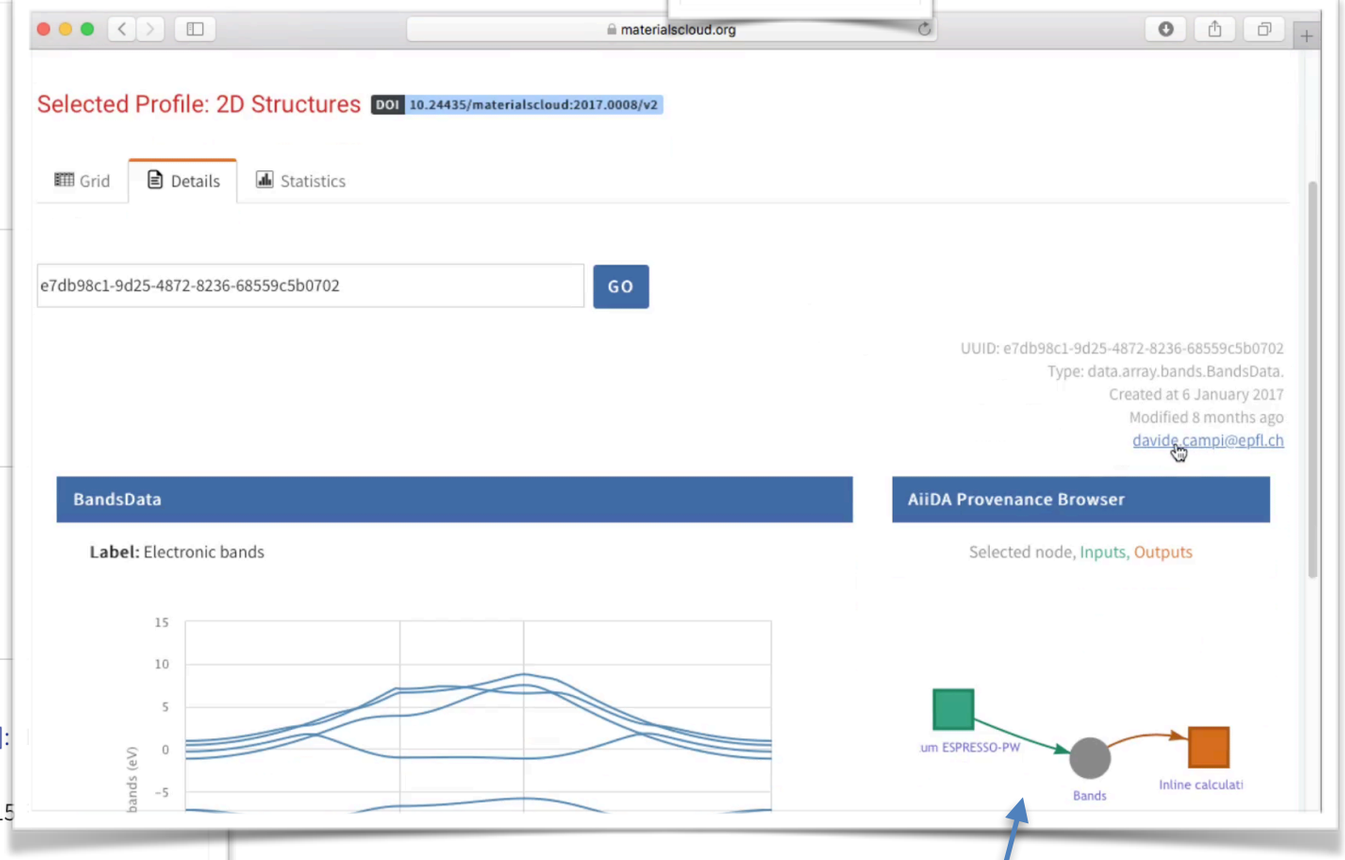

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DATA MANAGEMENT PLANS AND FAIR PRINCIPLES

- Combination of **AiiDA + Materials Cloud** (Discover, Explore, Archive): **FAIR-compliant sharing**

- **Findable**: DOIs with standardized metadata
- **Accessible**: web interface to browse data, calculations and provenance, curated data in Discover section
- **Interoperable**: data linked via the AiiDA directed graph; data structures reusable between different codes
- **Reusable**: downloadable data, encourage open (CC) licences, reproduce in the AiiDA Lab thanks to full provenance

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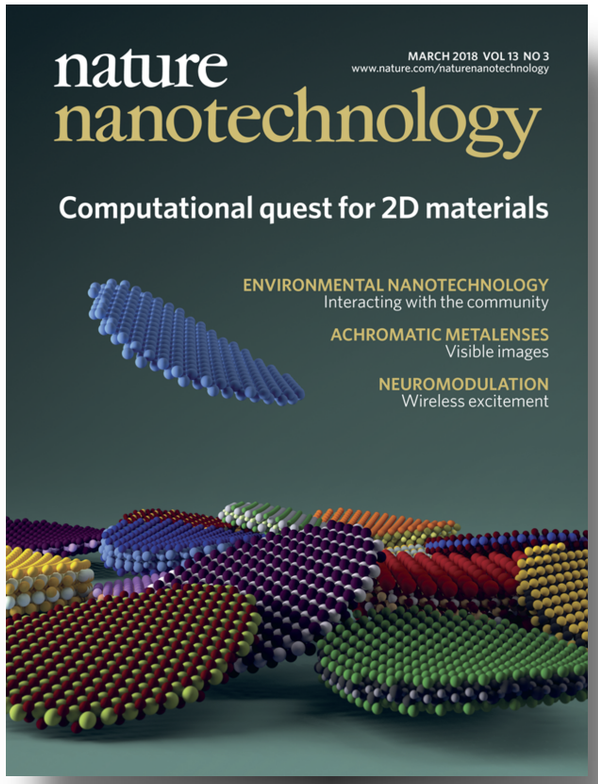
- We provide DMP templates for researchers using Materials Cloud (and we are coordinating with EMMC for a EU H2020 template)

Below, we provide templates for data management plans using the Materials Cloud Archive (with and without AiiDA).

Funding Body	DMP template (using AiiDA)	DMP template (no AiiDA)
SNF	.docx .odt .pdf	.docx .odt .pdf

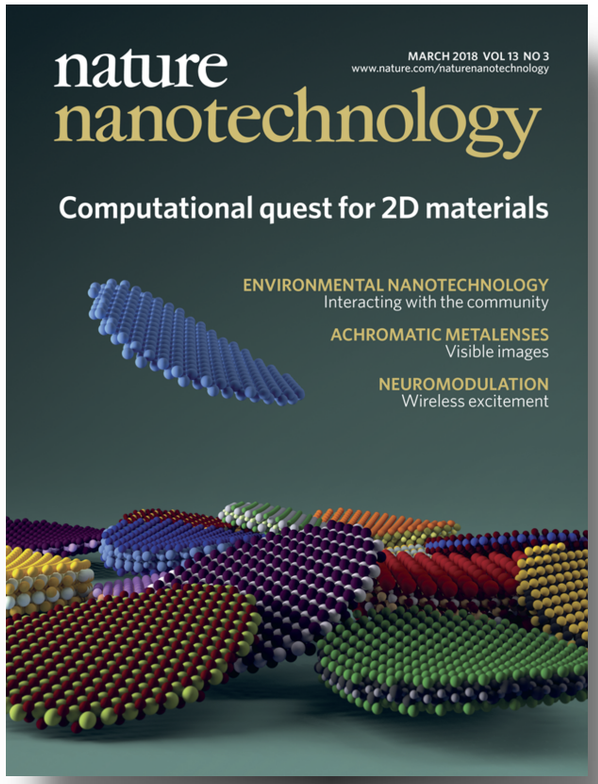
Open Data enables new research



N. Mounet et al.,
Nature Nanotech. 13, 246 (2018)

Data:
Nicolas Mounet et al.,
Materials Cloud Archive (2018),
10.24435/materialscloud:2017.0008/v2

Open Data enables new research



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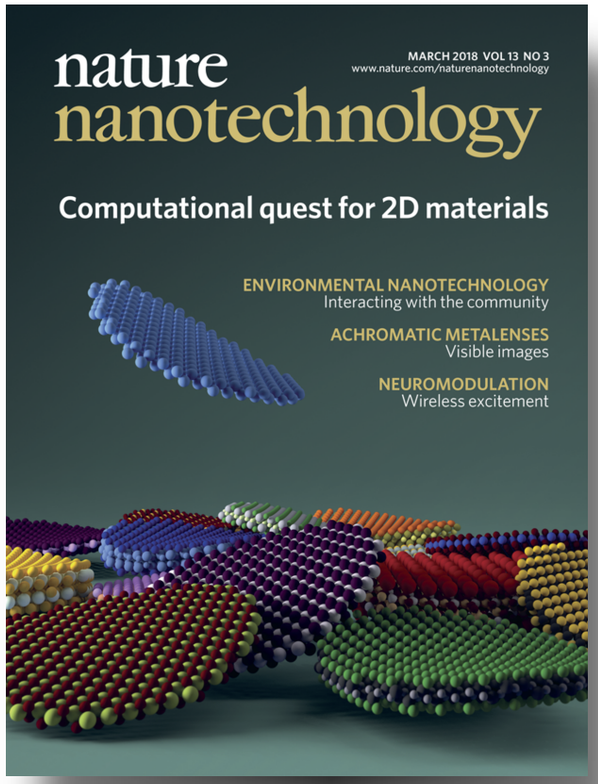
Data published on the
Materials Cloud
with **full provenance**
(as stored by AiiDA)

Open Data enables new research



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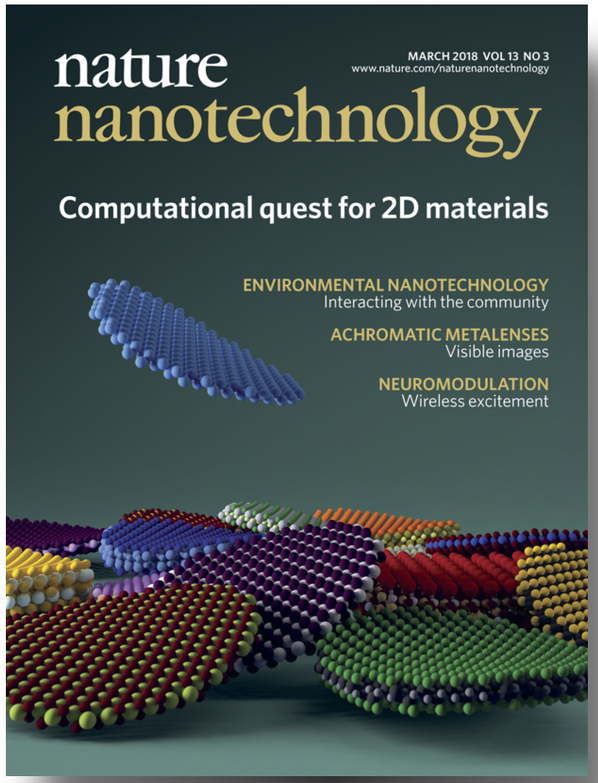
Groups at CINECA and University of Bologna: develop a project using the published data, with a **new unforeseen goal:**

Prediction of the absolute time per iteration of a Quantum ESPRESSO run

Open Data enables new research



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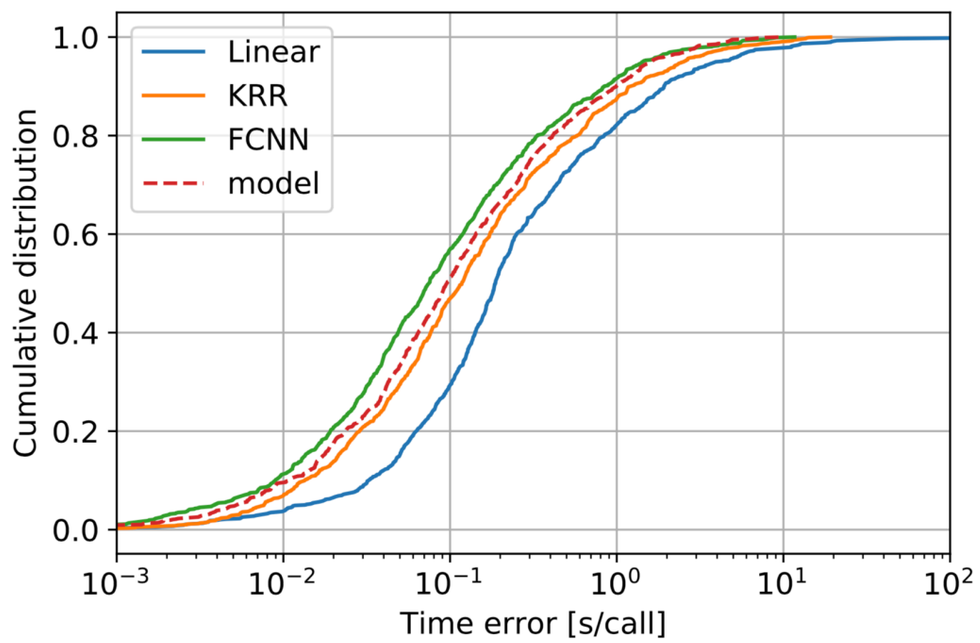


Groups at CINECA and University of Bologna: develop a project using the published data, with a **new unforeseen goal:**

Prediction of the absolute time per iteration of a Quantum ESPRESSO run

"Prediction of time-to-solution in material science simulations using

Deep Learning"

(accepted to PASC19)

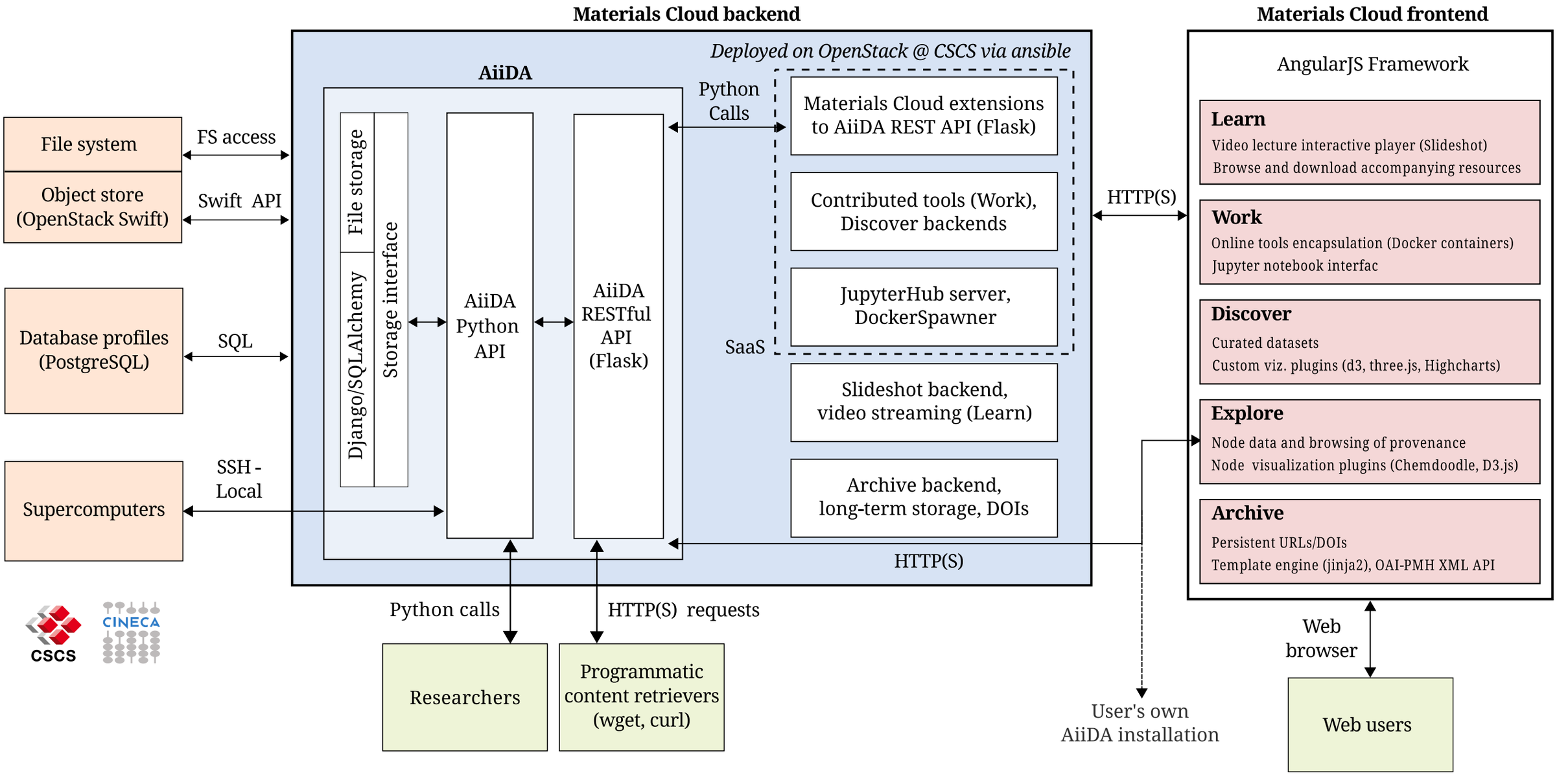
Need very detailed information on calculations, metadata, and machines ("identikeep")

ARCHIVE - FAQ

- Q: How much data can I upload per record?
  A: *Everyone:* 5GB regular, 50GB AiiDA.
  MARVEL & partners: for larger data sets just contact us
- Q: How long will it be stored?
  A: At least10 years after submission.
- Q: Can I update my record?
  A: Yes, but only references & keyword (otherwise: new version)
- Q: How to make a new version?
  A: Edit existing submission & request publication again
- Q: Can I *reserve* a DOI before publication?
  A: Not at the moment - we're working on it.

materialscloud.org/policies

THE ENTIRE PLATFORM



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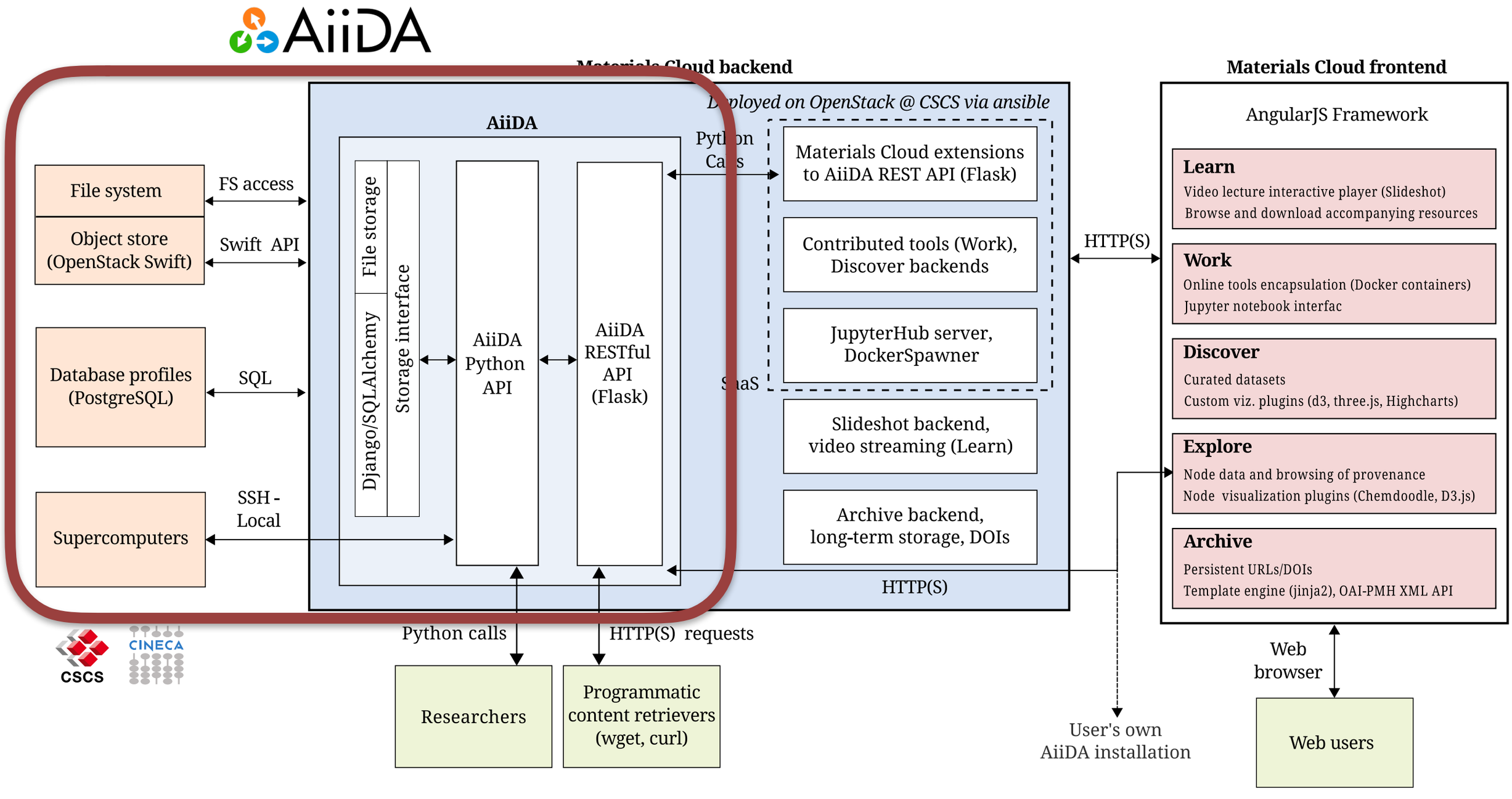
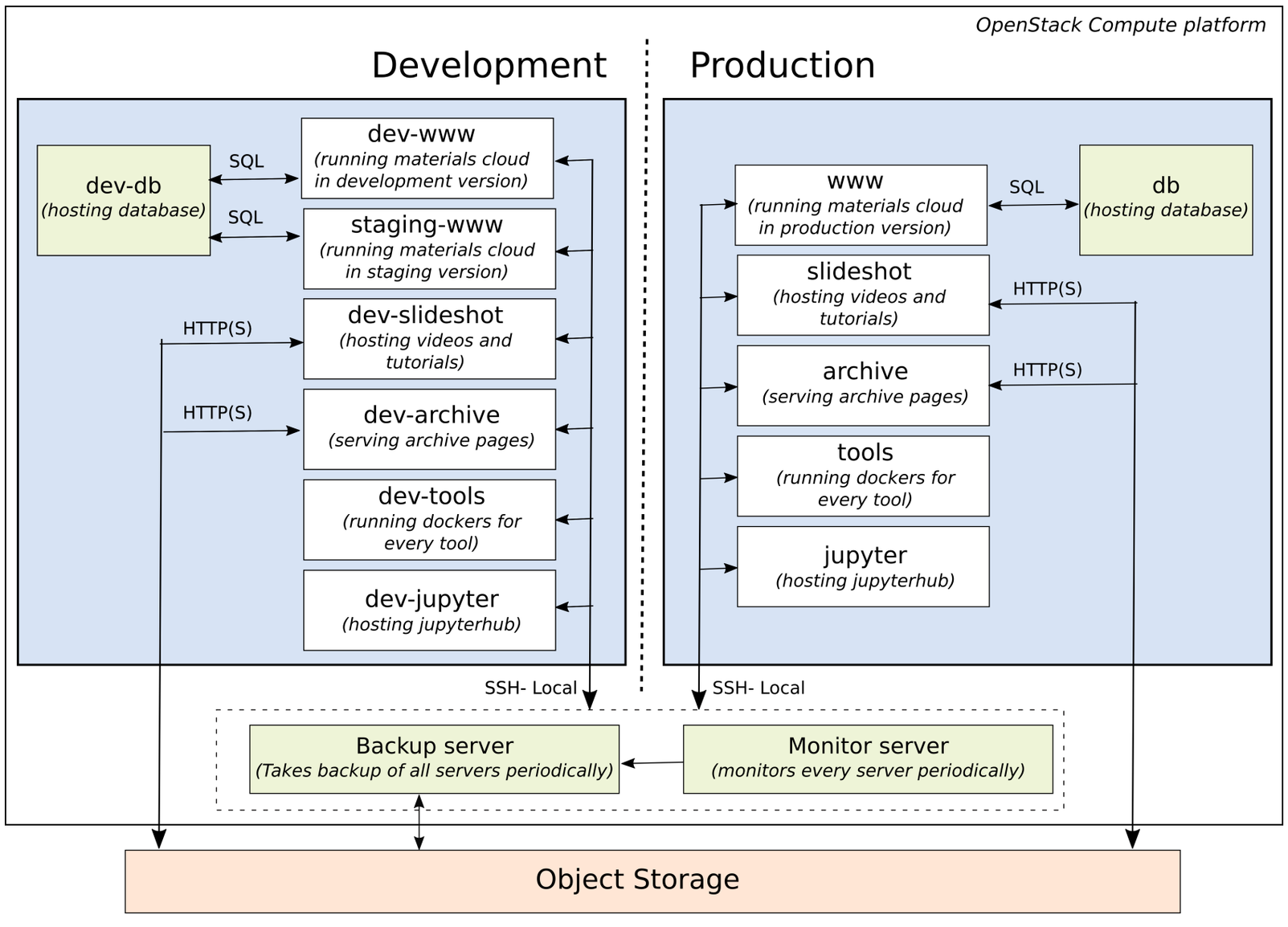


PLATFORM DEPLOYMENT



- Deployment on the OpenStack platform @ CSCS
- Managed with ansible
- 6 production VMs + monitor&backup servers
- Environment duplicated for development, ensuring stability
- Data stored on the object storage (Swift) and on the DB machines

Future plans

- Transition ARCHIVE to invenio 3
  - well-tested open-source software framework
  - scales up to millions of records (e.g. zenodo.org)
  - provides user management, search, serialization, …
- Scalable AiiDA lab
  - Using kubernetes, supporting 100+ users
  - Connected to existing authentication services
- Deploy AiiDA lab elsewhere
  - Companies and universities
  - **Contact us** if you want AiiDA lab in your institution!

Funding

- **SNSF MARVEL NCCR** (I: 2014-18, II:2018-22, EPFL Lead house)
  for the Open Science Platform
- **H2020 MaX Centre of Excellence** (I: 2015-18, II: 2018-21)
  for convergence of HPC, HTC and HPDA via AiiDA
- **H2020 MarketPlace** (2018-22, EPFL co-PI)
  for providing materials simulation services and data
- **H2020 Intersect** (2019-21, EU; CNR lead PI, EPFL and ICN2 co-PI)
  for automated modelling of complex devices via AiiDA
- Private collaboration with a **major European company** (2019-2020)
  for AiiDA-powered materials discovery for Li-ion batteries
- **Swissuniversities P-5 Materials Cloud** (2019-20)
  for transitioning Materials Cloud to self-sustaining service
- **EPFL Open Science Fund "OSSCAR"** (2019-21)
  for creating an educational hub for research and teaching

15+ FTEs for the next years