

NICOLA MARZARI, EPFL and PSI

THE RISE OF COMPUTATIONAL SCIENCE

A calculation that took one year in 1994 takes ten seconds in 2023: **3-million-fold increase, or 100% returns every 16 months.**

And this is just with bits: neurons are in, and qubits on the horizon. 21st-century science and discovery will greatly benefit from computational science.



THE RISE OF ELECTRONIC-STRUCTURE SIMULATIONS



THE TOP 100 PAPERS: 12 papers on densityfunctional theory in the top-100 most cited papers in the entire scientificmedical-engineering literature, ever.

NATURE, OCT 2014

THIS IS BIG SCIENCE... (APS, 2021)

Title	Authors	Journal	# cited
Generalized gradient approximation made simple	Perdew, Burke, Ernzerhof	PRL (1996)	108 099
Development of the Colle-Salvetti correlation-energy formula	Lee, Yang, Parr	PRB (1988)	77 473
Efficient iterative schemes for ab initio total-energy calculations	Kresse, Furthmüller	PRB (1996)	58176
Projector augmented-wave method	Blöchl	PRB (1994)	43 455
Self-consistent equations including exchange and correlation	Kohn, Sham	PR (1965)	42 795
From ultrasoft pseudopotentials to the projector augmented-wave	Kresse, Joubert	PRB (1999)	42 485
Special points for Brillouin-zone Integrations	Monkhorst, Pack	PRB (1976)	41 232
Density-functional exchange-energy approximation with correct	Becke	PRA (1988)	41 142
Inhomogeneous electron gas	Hohenberg, Kohn	PRB (1964)	35 445
Ab initio molecular dynamics for liquid metals	Kresse, Hafner	PRB (1993)	23 192

Table 1. Top ten most highly cited articles published by the American Physical Society, all of which deal with density functional theory and its practical application. Data collected from the Web of Science on June 16th, 2021.



...AND THIS IS THE FUNDING FOR BIG SCIENCE

- ESA **7.1 billion €/year** (2023)
- ITER **22 to 65 billion \$** (2007-35)
- CERN **1.4 billion CHF/year** (2023)
- Argonne **1.1 billion \$/year** (2021)
- James Webb **10 billion \$** (2021)







FORTUNE COOKIE

AGAINST SUCH MAJOR IMPACT, THERE IS RATHER MARGINAL FUNDING FOR THE INFRASTRUCTURE, AND NOT MUCH STRATEGY EITHER



2013 VISION

Materials Cloud is built to enable the seamless sharing and dissemination of resources in computational materials science, offering educational, research, and archiving tools; simulation software and services; and curated and raw data.



https://www.materialscloud.org

2013 VISION

- Moderated repository
- Long-term storage
- DOIs

•• EXPLORE

- Interactive graphs of AiiDA databases
- Raw data + provenance (inputs, outputs)

- Lecture recordings
- Tutorial videos, slides, course materials

% WORK

or on premises

- Simulation tools and services - AiiDAlab in the cloud
- Curated datasets
- Tailored visualizations

https://www.materialscloud.org

TARGET AUDIENCES

Section	Content	Target audience	Objective	Access	Submission
LEARN	Video lectures and tutorials	Students and experts in computational materials science	Dissemination of educational and research content	Open, no registration	Partners; other submissions considered
WORK	Online simulations tools and services; redeployable locally	Researchers in computational materials science	Dissemination of open simulation services and tools	Open, with registration for AiiDAlab	Partners; other submissions considered
DISCOVER	Curated datasets of calculated materials properties	Researchers in materials science	Dissemination of calculated materials properties	Open, no registration	Partners; other submissions considered
EXPLORE	AiiDA databases and their graphs	Researchers in computational materials science; data scientists	Exploration and query of the raw data and provenance of AiiDA workflows	Open, no registration	Open, with registration
ARCHIVE	Computational data in any format; experimental data linked to computational data	Researchers in materials science; data scientists	FAIR research data dissemination and storage	Open, no registration	Open, with registration



LEARN





BROAD ATTENDANCE

MARVEL Distinguished Lectures: Now fully online – great attendance worldwide (Kresse, 670 participants). E.g. 2021-22 Zunger, Perdew, Mertig, Glotzer, Aspuru-Guzik, Chan.



CECAM-MARVEL Classics in Molecular and Materials Modelling: 400-600 participants. For 2021-22:





https://www.materialscloud.org/learn/





MATERIALS CLOUD WORK

Work with your data

Tools and services for working with your data and generating new data in the cloud or directly on your machine.



DIRECTLY ACCESSIBLE TOOLS



UNIVERSAL APIs

https://optimadeclient.materialscloud.io/

https://www.materialscloud.org/work/tools/qeinputgenerator

14

OPTIMADE Open Databases Integration for Materials Design Currently valid OPTIMADE API version: v1.0.1 Client version: 2021.3.29 Source code: Cliftud Help improve the application: R Report a bug Suggest v This is a friendly client to search through databases and other img get more information about the OPTIMADE API, please see the O	Apply filters Basic Raw Chemistry Chemical Formula e.g., (H2O)2 Na Elements A Hida Exclodic Table Results Structures can include any chosen e H H Be Ascending id ✓ X4 Sort U Be Na Mg Co8Ge12Li12O48 (id=mp-1013807) ✓ Quantum	U 0.92489940900 0.11814340000 0.391340000 0.0.3926640000 0.318550000 0.0.4782280000 0.318550000 0.0.1973360000 0.5791910000 0.1755640000 0.0.9035650000 0.0217720000 0.3244360000 0.0.9035650000 0.0217720000 0.1181450000 0.0.5579191000 0.1755640000 0.107356000 0.0.8818550000 0.9782280000 0.8026640000 K_POINTS automatic 4.4.4.0.0.0 CELL_PARAMETERS angstrom -5.9308880000 5.9308880000 5.9308880000 5.9308880000 5.9308880000 -5.9308880000
OPTIMADE consortium's list of providers. Note: The structure property assemblies is currently not support > FAQ > Log Query a provider's database Select a provider Apply filters Basic Chemistry Chemisal Formula Elements A t Structures can include any chosen c	 k Ca Sc Ti V Cr Mn Fe Rb Sr Y Zr Nb Mo Tc Ru Cs Ba + Hf Ta W Re Os Fr Ra # Hf Db Sg Bh Hs La Ce Pr Nd Pm # Ac Th Pa U Np Number of Elements Cell Dimensionality Molecule Wire Planar Buil 	SPRESSO in B has been surse below and instance in case of frace
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IN THE CLOUD OR ON-PREMISES SIMULATIONS

m deployment (collaboration with **=** Micro https://github.com/aiidalab/aiidalab-k8s

AGILE DEPLOYMENT THROUGH THE QUANTUM MOBILE

THE DATA STRATEGY: ARCHIVE...

WORK DISCOVE	R EXPLORE ARCHIVE	
Q	About Submission instructions FAQs	Recommended by
		SCIENTIFIC DATA
Latest rec	ords	
		European
A robust framev	ork for generating adsorption isotherms to screen materials for carbon capture	Commission
Dol 10.24435/materials	laudha-aq d Mohamad Moosavi. Charithea Charalamhous. Susana Garcia. Berend Smit	Open Research Europe
In this paper, we pres	on monanical moderary, origination does of each a carbon control officiently predict, by using molecular simulations, the thermodynamic data that is needed to design a carbon capture process. We developed a procedure that does not rely on fitting of the ac	
obtain accurate data interested in low CO	or both, the pure component isotherms as well as the mixture isotherms. This allowed us to make a detailed comparison of the different methods to predict the mixture isotherms. All approaches rely on an accurate description of the pure component isotherms concentrations, it is essential that these models correctly, the dual-site Langmuir (DSL) model is often used for the pure compc	••
Latest version: v3		 Swiss National
Publication date: Jur	26, 2023	Science Foundation
Proximity-induc	ed Cooper pairing at low and finite energies in the gold Rashba surface state	Indexed by
DOI 10.24435/materials	loud:20-9z	
Philipp Rüßmann, Ma	soud Bahari, Stefan Blügel, Björn Trauzettel	
Multi-band effects in We explain both the superconducting pair	superconducting heterostructures provide a rich playground for unconventional physics. We combine two complementary approaches based on density-functional theory (DFT) and effective low-energy model theory in order to investigate the proximity effect in a (retical approaches and intertwine the effective model and DFT analysis. This allows us to predict finite energy superconducting avoided crossings due to the interplay of the Rashba surface state of Au, and hybrid zation with the electronic structure of super ng and analyze their mixed singlet-triplet character. Our findings demonstrate the general recipes to explore material systems that exhibit novel finite-energy pairings. This dataset accompanies a publication where the data is presented and discussed in detail.	regidata.org 🗾 🙆 🔘
Latest version: v1 Publication date: Jur	26, 2023	http://doi.org/10.17616/R32J5W V O
Pd-doping of Bi	Te₃ and superconductivity of Pd(Bi,Te) _x from density functional theory	
DOI 10.24435/materials	loud:4e-10	FAIRsharing.org
Philipp Rüßmann, Xia	n-Kui Wei, Abdur Rehman Jaliil, Yoichi Ando, Detlev Grützmacher, Stefan Blügel, Joachim Mayer	standards, databases, policies
Bi ₂ Te ₃ and Pd(Bi,Te), geometries for Pd int	(registrate zero modes gained a lot on attention in recent years due to the possibility to engineer topologically protected quantum computing platforms, Fromsing calculates are neterostructures of topological insulators and platforms and the superconducting protected quantum computing platforms, Fromsing calculates are neterostructures of topological insulators and platforms and the superconducting protected quantum computing platforms, Fromsing calculates are neterostructures of topological insulators and platforms and the superconducting plate when Pd is deposited on topological insulators and rester accompany and the superconducting plate when Pd is deposited on topological insulators and rester accompany and the superconducting plate when Pd is deposited on topological insulators and rester accompany and the superconducting plate when Pd is deposited on topological insulators and rester accompany and the superconducting plate when Pd is deposited on topological insulators and rester accompany and the superconducting plate when Pd is deposited on topological insulators and rester accompany and the superconducting plate when Pd is deposited on topological insulators and rester accompany and the superconducting plate when Pd is deposited on topological insulators and rester accompany and the superconducting plate when Pd is deposited on topological insulators and rester accompany and the superconducting plate set accompany and the superconducting plate when Pd is deposited on topological insulators and rester accompany and the superconducting plate set accompany and the supercon	
Latest version: v2 Publication date: Jur	22, 2023	
Oxygen reductio	n reaction on single-atom catalysts from density functional theory calculations combined with an implicit solvation model	
DOI 10.24435/materials		
Azim Fitri Ainul Abidi	, Ikutaro Hamada	
We present a density comparable ORR active reaction free energies	functional theory study of the oxygen reduction reaction (ORR) on a single atom catalyst embedded in graphene, namely, TM-N ₄ -C (TM = Fe and Co), using the effective screening medium method combined with the reference interaction site model (ESN vities from the constant electode potential simulations, in contrast to the results obtained using the constant (neutral) charge simulation, in which the superior performance of Co-N ₄ -C has been predicted. The constant charge devices the constant charge simulation of the elector in the constant charge devices the included as an ad hoc maner. We success the importance of the variable charge in the simulation of the elector. The constant charge to SC -N ₄ -C has been predicted. The constant charge to SC -N ₄ -C has been predicted. The constant charge to SC -N ₄ -C has been predicted by SEM-FISM.	Google
Latest version: v1 Publication date: Jur	22, 2023	
First-principles	tudy of the gap in the spin excitation spectrum of the Crl₃ honeycomb ferromagnet	Collaborative
DOI 10.24435/materials	loudrb-24	EUDAT Data Infrastructure

Tommaso Gorni, Oscar Baseggio, Pietro Delugas, Iurii Timrov, Stefano Baroni

Open "https://archive.materialscloud.org" in a new tab a gap observed at the zone border in the spin excitation spectrum of Crl3 quasi-two-dimensional single crystals is still controversial. We perform first-principles calculations based on time-dependent density functional perturbation theory, which indicate that the observed or

THE DATA STRATEGY: ...DISCOVER...

Discover curated data sets

Curated research data sets with tailored visualizations maintained by the Materials Cloud team.

Materials Cloud three-dimensional crystals database (MC3D) DOI 10.24435/materialscloud

Authors: Sebastiaan Huber, Marnik Bercx, Kristjan Eimre, Nicolas Hörmann, Martin U Marzari, Giovanni Pizzi

Description: Curated set of relaxed three-dimensional crystal structures based on raw from the experimental databases MPDS, COD, and ICSD.

DOI 10.24435/materialscloud:36-nd

Authors: Davide Campi, Davide Grassano, Nicolas Mounet, Marco Gibertini, Philippe Andrius Merkys, Antimo Marrazzo, Thibault Sohier, Ivano E. Castelli, Andrea Cepellotti Kumbhar, Elsa Passaro, Kristjan Eimre, Giovanni Pizzi, Nicola Marzari

Materials Cloud two-dimensional crystals database (MC2D) DOI 10.24435/materialscloud:az

Description: Results from screening known 3D crystal structures finding those that ca computationally exfoliated, producing 2D materials candidates.

Standard solid-state pseudopotentials (SSSP) DOI 10.24435/materialscloud:rz-77

Authors: Gianluca Prandini, Antimo Marrazzo, Ivano E. Castelli, Nicolas Mounet, Sne Elsa Passaro, Nicola Marzari

Description: A Standard Solid State Pseudopotentials (SSSP) library optimized for pre efficiency.

Verification of the precision of DFT implementations via AiiDA common workflows

DOI 10.24435/materialscloud:s4-3h

Authors: E. Bosoni, L. Beal, M. Bercx, P. Blaha, S. Blügel, J. Bröder, M. Callsen, S. C. Degomme, V. Dikan, K. Eimre, E. Flage-Larsen, M. Fornari, A. Garcia, L. Genovese, M Giantomassi, S. P. Huber, H. Janssen, G. Kastlunger, M. Krack, G. Kresse, T. D. Kühn-Lejaeghere, G. K. H. Madsen, M. Marsman, N. Marzari, G. Michalicek, H. Mirhosseini, Müller, G. Petretto, C. J. Pickard, S. Poncé, G. Rignanese, O. Rubel, T. Ruh, M. Sluyd! Vanpoucke, S. Vijay, M. Wolloch, D. Wortmann, A. V. Yakutovich, J. Yu, A. Zadoks, B.

Description: Reference and verification datasets of equations of state calculated with superind density-functional-theory (DFT) codes and computational approaches, using the AiiDA common workflows (ACWF) infrastructure.

Materials Cloud three-dimensional crystals database (MC3D)

DOI 10.24435/materialscloud:rw-t0

Curated set of relaxed three-dimensional crystal structures based on raw CIF data from the experimental databases MPDS, COD, and ICSD.

Use About REST API

Search for materials:

THE DATA STRATEGY: ...DISCOVER...

THE DATA STRATEGY: ... EXPLORE

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INTEROPERABILITY: FROM ARCHIVE TO IN-CLOUD ANALYSIS

INTEROPERABILITY: ON-PREMISES SIMULATIONS

Quantum ESPRESSO input generator, or full simulations services in AiiDAlab

Quantum ESPRESSO input generator and structure visualizer

•	About the Quantum ESPRESSO input generator and st	tructure visualizer
-	Instructions	
-	Acknowledgements	
Up	load your structure	
	Upload a crystal structure: Select here the file format: Select here the pseudopotential library: Select here the magnetism/smearing: ^[?] Select here the k-points distance (1/Å) ^[?] (and smearing (eV) in case of fractional occupations): Refine cell (using spglib):	Choose File NO file SE Cted Quantum ESPRESSO into [parser: qetools] C SSSP Efficiency PBEsol (version 1.1) C Intervention non-magnetic metal (fractional occupations) C Intervention fine (0.20 1/Å, 0.2 eV) C C No C C C
	By continuing, you agree	e with the terms of use of this service.
	Generate	∋ the PWscf input file

Otherwise, pick an example

Select here a structure:	AI 🖸
Select here the pseudopotential library:	SSSP Efficiency PBEsol (version 1.1) 📀
Select here the magnetism/smearing:[?]	non-magnetic metal (fractional occupations) 🔅
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(and smearing (eV) in case of fractional occupations):	
By continuing, you agree with	the terms of use of this service.
Operate the D	
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INTEROPERABILITY: INTEGRATION WITH MATERIALS CLOUD TOOLS

Summary of the input parameters

Pseudopotential library: SSSP Efficiency PBEsol (version 1.1)

Smearing/magnetism: non-magnetic metal (fractional occupations)

K-points distance: 0.2 Å⁻¹

The input parameters provided by this tool are accurate safe choices. Optimized choices that allow for faster runs with comparable accuracy can be achieved by expert users.

Additionally, the input file provided here does not guarantee that the Quantum ESPRESSO calculation will always converge successfully. Indeed, this is just the first step of the automated workflows released within the alida-quantum spresso package. These implement advanced strategies to reduce the failure rate of the code by changing the input parameters to achieve convergence.

If you don't have AiiDA installed, you can anyway try out the workflows inside the Quantum Mobile virtual machine, by using the "Quantum ESPRESSO" app inside the AiiDAlab interface.

If you use the results of this tool in a publication, please cite the following works:

- SSSP (for the pseudopotential library)
 G. Prandini, A. Marrazzo, I. E. Castelli, N. Mounet and N. Marzari, npj Computational Materials 4, 72 (2018).
 WEB: http://materialscloud.org/sssp.
- Pseudopotentials:
- bi_pbesol_v1.uspp.F.UPF,
- cl_pbesol_v1.4.uspp.F.UPF,
- s_pbesol_v1.4.uspp.F.UPF,

from <u>GBRV</u>: K. F. Garrity, J. W. Bennett, K. M. Rabe, and D. Vanderbilt, *Comput. Mater. Sci.* 81, 446 (2014). DOI: 10.1016/j.commatsci.2013.08.053, WEB: http://www.physics.rutgers.edu/gbrv, LICENSE: GNU General Public License (version 3).

- Ag_ONCV_PBEsol-1.0.upf,
- from SG15: M. Schlipf and F. Gygi, Comp. Phys. Comm. 196, 36 (2015).

DOI: 10.1016/j.cpc.2015.05.011, WEB: http://www.quantum-simulation.org/potentials/sg15_oncv, LICENSE: Creative Commons Attribution-ShareAlike 4.0 International License (CC BY-SA 4.0).

- Al.pbesol-n-kjpaw_psl.1.0.0.UPF,
- from Pslibrary 1.0.0: A. Dal Corso, Comput. Mater. Sci. 95, 337 (2014).

DOI: 10.1016/j.commatsci.2014.07.043, WEB: http://www.quantum-espresso.org/pseudopotentials, LICENSE: GNU General Public License (version 2 or later).

🛓 Download zip of input file and pseudopotentials 🛛 🖸 Change parameters 🗎 🛓 Choose a different structure

Quantum ESPRESSO PWscf input

Sopy to clipboard

```
&CONTROL
    calculation = 'scf'
    etot_conv_thr = 3.400000000d-04
    forc_conv_thr = 1.000000000d-04
    outdir = './out/'
    prefix = 'aiida'
    pseudo_dir = './pseudo/'
    tprnfor = .true.
    tstress = .true.
    verbosity = 'high'
    /
    &SYSTEM
    degauss = 1.4699723600d-02
    ecutrho = 3.600000000d+02
```


INTEROPERABILITY: INTEGRATION WITH MATERIALS CLOUD TOOLS

Summary of the input parameters

Pseudopotential library: SSSP Efficiency PBEsol (version 1.1)

Smearing/magnetism: non-magnetic metal (fractional occupations)

K-points distance: 0.2 Å⁻¹

The input parameters provided by this tool are accurate safe choices. Optimized choices that allow for faster runs with comparable accuracy can be achieved by expert users.

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 G. Prandini, A. Marrazzo, I. E. Castelli, N. Mounet and N. Marzari, npj Computational Materials 4, 72 (2018).
 WFB: http://materialsclud.org/ssso.
- Pseudopotentials:
- bi_pbesol_v1.uspp.F.UPF,
- cl_pbesol_v1.4.uspp.F.UPF,
- s_pbesol_v1.4.uspp.F.UPF,

from <u>GERV</u>: K. F. Garrity, J. W. Bennett, K. M. Rabe, and D. Vanderbilt, *Comput. Mater. Sci.* **81**, 446 (2014). DOI: 10.1016/j.commatsci.2013.08.053, WEB: http://www.physics.rutgers.edu/gbrv, LICENSE: GNU General Public License (version 3).

Ag_ONCV_PBEsol-1.0.upf,

from <u>SG15</u>: M. Schlipf and F. Gygi, *Comp. Phys. Comm.* **196**, 36 (2015). DOI: 10.1016/j.cpc.2015.05.011, WEB: http://www.quantum-simulation.org/potentials/sg15_oncv, LICENSE: Creative Commons Attribution-ShareAlike 4.0 International License (CC BY-SA 4.0).

Al.pbesol-n-kjpaw_psl.1.0.0.UPF,

from Pslibrary 1.0.0: A. Dal Corso, Comput. Mater. Sci. 95, 337 (2014).

DOI: 10.1016/j.commatsci.2014.07.043, WEB: http://www.quantum-espresso.org/pseudopotentials, LICENSE: GNU General Public License (version 2 or later).

🗄 Download zip of input file and pseudopotentials 🛛 🗹 Change parameters 🛛 🏝 Choose a different structure

Quantum ESPRESSO PWscf input

Sopy to clipboard

&CONTROL calculation = 'scf' etot_conv_thr = 3.4000000000d-04 forc_conv_thr = 1.0000000000d-04 outdir = ',/out/' prefix = 'aiida' pseudo_dir = ',/pseudo/' tprnfor = .true. tstress = .true. verbosity = 'high' / &SYSTEM degauss = 1.4699723600d-02 ecutrho = 3.600000000d+02

ecutwfc = 5.000000000d+01

AiiDAlab

Å AiiDAlab

AIIDAab provides you with a dedicated and intuitive simulation environment directly in the cloud or on remote or local resources. With AIIDAab you can nu and manage complex, robust, and reliable workflows with tailored lightweight web applications, all from your browser. In addition, you can easily create your own applications, all running on top 01AIDA workflows.

File Manager Terreted Tasks App Store Holp

Features

A cloud platform where you launch and monitor AIIDA workflows, and analyze the results.
 Dedicated applications with intuitive graphetal user interfaces.
 Sharing of aps and workflows with the AIJAblab APS Store.
 A. Fast development of new apps as Juryter notebooks.
 S. Open technologies throughout: I notis your own AIIDAtablab

Publication

We kindly ask you to cite the following publication if you use AiiDAlab A. V. Yakutovich et al., Comp. Mat. Sci. 188, 110165 (2021). DOI:10.1016/j.commatsci.2020.110165

Documentation

AiiDAlab documentation can be found on the following web page. Apps

The list of available apps can be found at the AiiDAlab App Store Open Source

AiiDAlab is open source. We invite you to explore the repositories in our GitHub organization.

Official deployments

 Status
 Login
 Description & Access policies

 UP
 Login
 Open AiiDAlab demonstrator running on the kubernetes cluster hosted at CESNET (under a EOSC

OpenStack cluster hosted at the Swiss National Supercomputing Centre (CSCS) under a FENIX grant (production instance)

Additionally, you can host AiiDAlab yourself on-premises or in the cloud (see the documentation).

Testimonials

Read the Interview with Dr. Carlo A. Pignedoli from Empa, describing how AliDAlab is used in a mixed theoretical/experimental research group.

For more information and feedback on AliDAlab, please contact alidalab@materialscloud.or

INTEGRATION WITH THE EUROPEAN COMMISSION

Cloud simulations

***	Cont	act us Portal Home	Catalogue & Marketplace	Providers Dashboard Login
EUROPEAN I SCIENCE CL	PEN Find resource		All resour V Q	My EOSC Marketplace
Resources → Access physical & el	frastructures > Compute > Other > AiiDAlab			
AiiDAlab	AiiDAlab Reproducible turn-key workflows for materials science Organisation: Materials Cloud		Access	the resource
	☆☆☆☆☆ (0.0 /5) 0 reviews ☐ Add to comparison → Webpage → Helpdesk e-mail → Manual → Training	g information	Ask a question	about this resource?
ABOUT DETAILS	REVIEWS (0)			
A is a workflow manager for	omputational science with a strong focus on provenance and per	rformance. Through its f	lexible SCIENTIFIC	CATEGORISATION
ramming language, and auto and manage AiiDA-powered v s from the application registr	a more range or simulation code and makes driven available role in matcally records the full provenance of your simulation pipeline rorkflows through tailored web applications in the browser. Use I or write your own in just a few lines of python using jupyter wid or compared to the tail of the MARVEL National Centre for Compet-	in a graph. AiiDAlab lets the App store to pick and lgets and appmode. This ence in Research, the Fu	s you d install service	es
20 MarketPlace project, by sv	issuniversities as well by a number of other partners.	ence in rescarch, the Eu	Natu	ral Sciences

https://marketplace.eosc-portal.eu/services/aiida-lab

Repository and long-term storage

MATERI		Materials Cloud Archive A long-term FAIR data repository for computational materials science Organisation: Materials Cloud	Access the resource
ABOUT	DETAILS	→ Webpage → Helpdesk e-mail → Manual REVIEWS (0)	Ask a question about this resource?
The Materials (allows research least 10 years) accessibility via and relevance	Cloud Archive is a ners worldwide to of data records a I standard protoc to the field of ma	n open-access, moderated repository for research data in computational materials science, that upload and publish their data free of charge. The repository guarantees long-term storage (for at nd associated metadata, their findability via persistent identifiers (including a DOI), and their ols. Submissions are moderated to ensure their completeness, adherence to the FAIR principles, terials science. This service is supported by a number of partners.	SCIENTIFIC CATEGORISATION Natural Sciences

https://marketplace.eosc-portal.eu/services/materials-cloud-archive

Country Sheets Analysis

Example of good practice

HPC and EOSC collaboration and training

Materials design at eXascale (MAX) is currently collaborating with EOSC and has already participated in key events throughout 2019, including the EOSC-hub Week. Such tools as AiiDA and Materials Cloud Archive are paving the way for new computational materials science and for granting streamlined access to HPC. MAX also performs tutorials using Virtual Machines, in particular the Quantum Mobile.

Available at https://archive.big-map.eu/

ACCESS AND STATISTICS

- 16,000 unique visitors monthly; 2,500 to the Archive
- No cookies, all open access

MATERIALS CLOUD DEPLOYMENT

L. Talirz *et al.,* Scientific Data 7, 299 (2020)

CONCLUSIONS – THE NEED FOR DIGITAL INFRASTRUCTURES

- Computational science is central to the entire scientific and technological effort in the 21st century – no other enabler can compete in terms of speed and acceleration
- Not many policymakers, or even the scientific community at large, have understood its structural needs, and long-term opportunity
- As a side note, it is a powerfully democratic force, that can be shared worldwide at the flick of a switch.

BROADER FINAL THOUGHTS

- Switzerland could do a fantastic job in leveraging competencies and resources if we move from
 Institution-wide efforts to domain-wide efforts i.e., not having an EPFL, an ETHZ, a PSI, etc...
 repository, but flagship efforts on domains (synchrotron, XPS, catalysis, planets, computational, etc...).
 This is what the community needs having data on the same topic fragmented across institutions
 makes them rarely useful or usable.
- Data can be shown to be valuable when others feel the need to use those curation and accessibility are key. Raw experimental and computational data without extensive curation are useless. Key is:
 - to develop "universal" domain-specific APIs that can be used to interrogate repositories across institutions/centres/etc... - these are agreed upon by experts in a domain, and ideally engaging international groups like the research data alliance (RDA) or at least key european players.
 - to insist on curation of data, where these are accompanied by extensive material that makes it usable, if in a niche domain, or using standard protocols if in a flagship domain
 - people will happily contribute to a domain-wide repository, but if it's institution-wide it will remain a niche effort. I would strongly suggest to pool resources across institutions, and consider opening our repositories to the wider community. In many endeavours the cost is the personnel, not the data storage (in other, linked to major facilities, is the opposite)

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Core Developers

Dou Du

epfl.ch

Materials, EPFL

PostDoc Web Engineer, Theory and Simulation of

PostDoc Research Scientist, Laboratory of

Computational Science and Modelling, EPFL

Roberto Bendinell Software developer, CECAM & Theory and Simulation of Materials, EPFL

epfl.ch

epfl.ch

Kristian Eimre PostDoc Web Engineer, Theory and Simulation of Materials, EPFL epfl.ch

Valeria Granata PostDoc Web Engineer, Theory and Simulation of Materials, EPFL epfl.ch

psi.ch

Xing Wang PostDoc, Materials Software and Data Group, PSI

Aliaksandr Yakutovich

Giovanni Pizzi Group leader. Materials Software and Data Group. PSI psi.ch

ethz.ch, cscs.ch

Joost VandeVondele Associate Director, Swiss National Supercomputing Center, CSCS

Deputy Group Leader, nanotech@surfaces laboratory, Empa empa.ch

Executive Committee

The Executive Committee of Materials Cloud is currently formed by:

- Kristjan Eimre (EPFL, Switzerland) [2022-] (representative of the Materials Cloud developers)
- Sara Bonella (EPFL and CECAM, Switzerland) [2020-]
- Carlo Pignedoli (Empa, Switzerland) [2020-]
- Nicola Marzari (EPFL, Switzerland) [2018-]
- Elisa Molinari (Unimore and CNR Nano, Italy) [2018-]
- Giovanni Pizzi (PSI, Switzerland) [2018-]
- Berend Smit (EPFL, Switzerland) [2018-]
- Joost VandeVondele (ETHZ and CSCS, Switzerland) [2018-]
- Tejs Vegge (DTU, Denmark) [2020-]

Materials Cloud@HPC Board

The Materials Cloud@HPC Board, created in late 2020, is currently formed by:

- Fabio Affinito (CINECA, Italy)
- Pekka Manninen (CSC, Finland)
- Giovanni Pizzi (PSI, Switzerland) (Materials Cloud representative)
- Dirk Pleiter (JSC, Germany)
- Joost VandeVondele (CSCS, Switzerland)

empa.ch

Jusong Yu PostDoc, Materials Software and Data Group, PSI psi.ch

FUNDING

http://theossrv1.epfl.ch Theory and Simulation of Materials (2011 onwards)

<u>http://nccr-marvel.ch</u> Swiss National Centre for Computational Design and Discovery of Novel Materials (2014-26)

http://max-centre.eu H2020 Centre of Excellence MaX: Materials Design at the Exascale (2015-26)

https://www.psi.ch/en/lms Laboratory for Materials Simulations (2021 onwards)

<u>https://www.big-map.eu</u> H2020 Battery Interface Genome – Materials Acceleration Platform (Battery 2030+, 2020-23, ...)

> https://www.uni-bremen.de/mapex U Bremen Excellence Chair (2018-25)

H2020 Nanoscience Foundries and Fine Analysis H2020 European Materials Modelling Council H2020 Marketplace H2020 Intersect H2020 DOME 4.0 H2020 OpenModel H2020 NEP DOME 4.0 H2020 EPFL Fellows H2020 EPFL Innovators H2020 Marie Curie SOLVAY **EPFL Open Science NCCR Catalysis** n Model MarketPlace PASC PRACE RICHEMONT Constellium TERSECT IBM **Robert Bosch Stiftung** Innosuisse **1913 191 Robert Bosch StiftungSolvay** Samsung SAMSUNG **Richemont Varinor** eu .eu