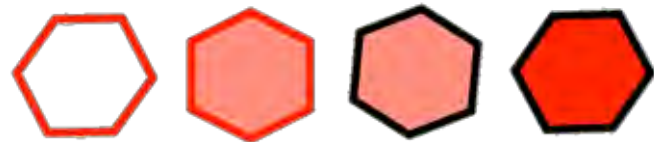

STRATEGIC AREAS

MARVEL

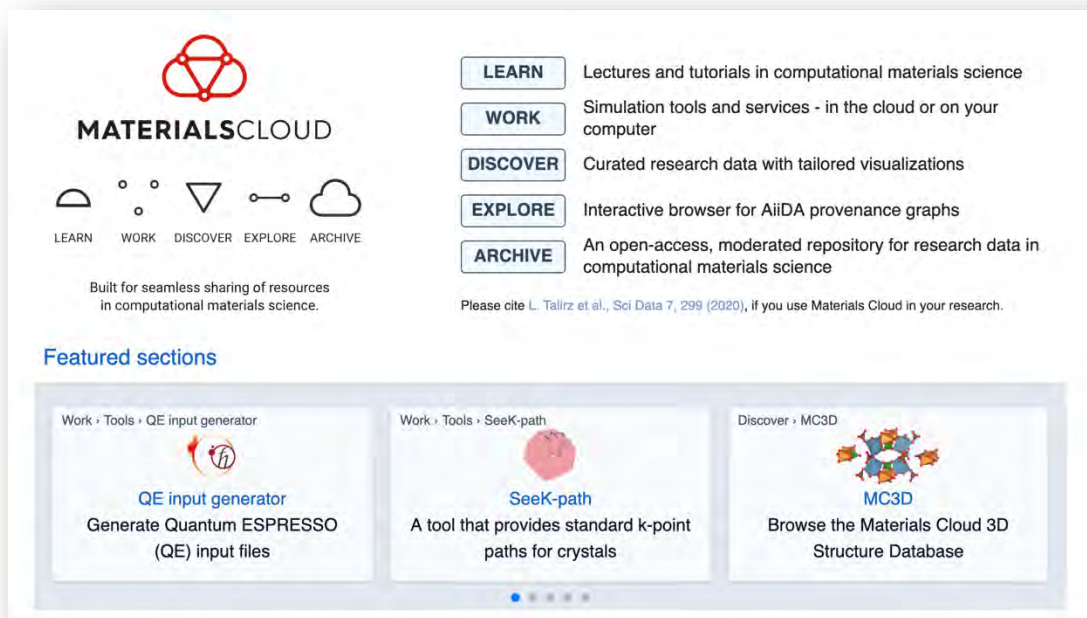


NATIONAL CENTRE OF COMPETENCE IN RESEARCH

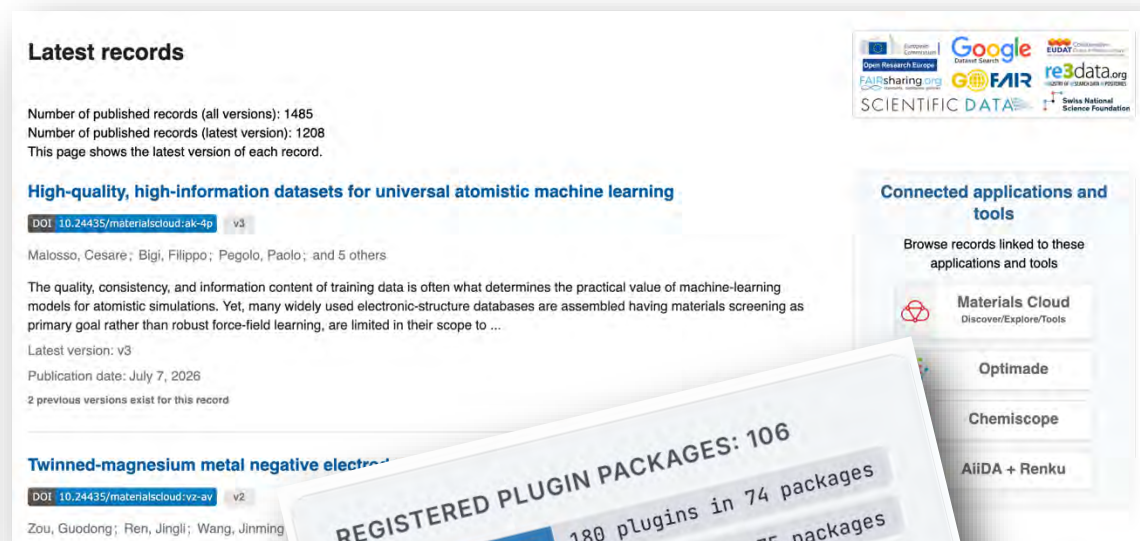


KTT: THE OPEN-SOURCE DIGITAL INFRASTRUCTURE

Open-source infrastructure as MARVEL's main transfer vehicle - Materials Cloud, AiiDA/AiiDALab, and Quantum Mobile as the main KTT success: **20,000+ unique visitors/months, 106 plugin packages and 200+ workflows. Embedded into MaX and CECAM.**



The Materials Cloud homepage features a navigation bar with icons for LEARN, WORK, DISCOVER, EXPLORE, and ARCHIVE. Below the navigation bar, there are five main sections: LEARN (Lectures and tutorials in computational materials science), WORK (Simulation tools and services - in the cloud or on your computer), DISCOVER (Curated research data with tailored visualizations), EXPLORE (Interactive browser for AiiDA provenance graphs), and ARCHIVE (An open-access, moderated repository for research data in computational materials science). A citation for L. Tallir et al., Sci Data 7, 299 (2020) is provided. The featured sections include: QE input generator (Generate Quantum ESPRESSO (QE) input files), Seek-path (A tool that provides standard k-point paths for crystals), and MC3D (Browse the Materials Cloud 3D Structure Database).



The Materials Cloud record page displays the latest records, including the number of published records (all versions: 1485, latest version: 1208). It highlights a high-quality, high-information dataset for universal atomistic machine learning, with a DOI of 10.24435/materialscloud:ak-4p v3. The record is attributed to Malosso, Cesare; Bigi, Filippo; Pegolo, Paolo; and 5 others. The page also lists connected applications and tools, including Materials Cloud, Optimade, Chemiscope, and AiiDA + Renku.

REGISTERED PLUGIN PACKAGES: 106

Category	Count
Calculations	180 plugins in 74 packages
Parsers	155 plugins in 75 packages
Data	133 plugins in 41 packages
Workflows	242 plugins in 52 packages
Console scripts	43 plugins in 21 packages
Other	122 plugins in 34 packages



Open-source infrastructure as MARVEL's main transfer vehicle – More than 40 open-source codes



Swiss National
Science Foundation



KTT: IAB, INDUSTRY SECTOR DAYS

- Industrial Advisory Board to engage in technology transfer
- Industry Sector Days on 1) metals, 2) chemicals/catalysis, 3) ICT, 4) energy, 5) pharma.
- Collaborations with companies - Solvay, Samsung, Bosch, Gaznat, Microsoft, BASF and Materials Design.



KTt: INDUSTRY DAY

2024 Empa Industry Day drew about 100 participants and speakers from IBM, BASF, Bosch, Microsoft, Schott and Beyond Gravity.

MARVEL Industry Day @Empa

Sep 05, 2024, from 9:00 until 17:00, Empa-Akademie, Dübendorf



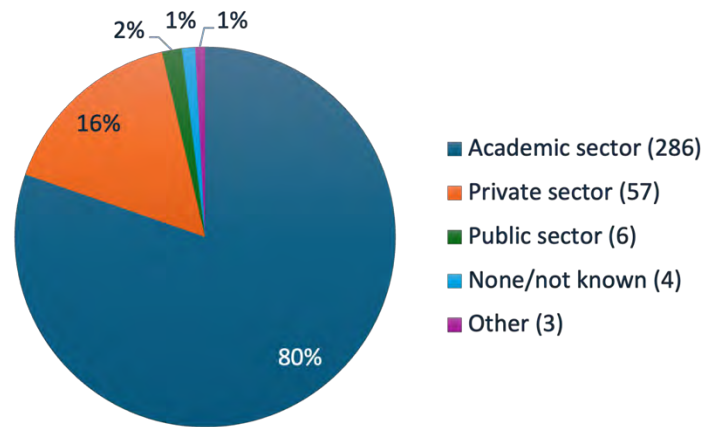
Program

- 09:00 — Welcome coffee
- 09:30 — Introduction, NCCR MARVEL Overview and MARVEL Industrial engagement
- 10:00 — **Keynote lecture : Prof. Roberto Car** (Princeton University): *Coarse-graining ab-initio molecular dynamics with machine learning*
- 10:30 — Discussion
- 10:45 — **Ivano Tavernelli** (IBM): *Quantum computing in the utility era*
- 11:05 — Discussion
- 11:15 — **Edvin Fako** (BASF): *Heterogenous catalyst design: High throughput experiments and machine learning accelerated high throughput simulations*
- 11:35 — Discussion
- 12:00 — Lunch + Poster Session
- 13:30 — **Maximillian Amsler** (Bosch): *Advancing through classical and quantum computing at Bosch*
- 13:50 — Discussion
- 14:00 — **Loris Ercole** (Microsoft Azure Quantum): *Accelerating computational materials discovery with Azure Quantum Elements*
- 14:20 — Discussion
- 14:30 — **Marco Ravasi** (Empa with Beyond Gravity): *Launch vehicle vibration attenuation through large-scale phononic crystal inspired arrangements*
- 14:50 — Discussion
- 15:00 — Coffee break
- 15:15 — **Leopold Talirz** (Schott): *Computational materials engineering at Schott*
- 15:35 — Discussion
- 15:45 — **Ivan Shorubalko** (Empa): *Colloidal quantum dots based photodetectors: materials, technology, concepts, architectures, performance, sustainability*
- 16:05 — Discussion
- 16:15 — **Panel Discussion**
- 17:00 — Final remarks and conclusion

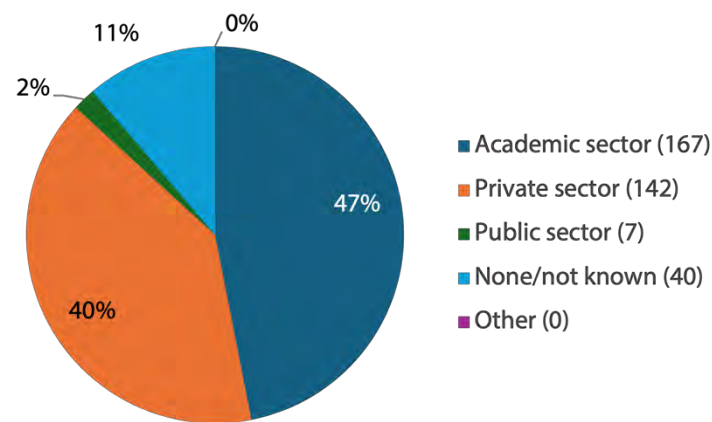


KTT: TRANSFER PEOPLE AND KNOW-HOW TO INDUSTRY

People as the most effective technology-transfer channel. The strongest transfer mode was trained people moving into industry: **57 junior researchers** transitioned directly to the private sector after MARVEL, and by spring 2026 about **40%** of former MARVEL PhD students and postdocs were in the private sector.



Next employer



Current employer in spring 2026

From MARVEL to industry

Many former members of our consortium have moved to the industry after working as PhD students or postdocs in one of the MARVEL laboratories. From ICT to energy, from chemical engineering to automotive, several industry sectors value the skills and competences that can be developed doing research on computational materials science. In this section, we talk to some former MARVEL members who are now working in the private sector, to know more about their experience and the advice they have for younger researchers who are interested in careers beyond academia.

The list is not exhaustive and new interviews will be added regularly.

- **Leopold Talirz**, formerly with Berend Smit's laboratory at EPFL, moved to Senior Software Engineer in the Azure Quantum team at Microsoft.
- **Giulia Mangione** worked in Clémence Corminboeuf's group at EPFL, and moved to Design Tech Lead at Stellantis.
- **Leonid Kahle** was a PhD and then postdoc in Nicola Marzari's lab, and moved to Materials Design Inc, a company specializing in atomistic simulation software.
- **Sandip De** worked with Michele Ceriotti at EPFL from 2015 to 2018, and then lead a team working on quantum mechanical simulation at BASF.
- **Chiara Ricca**, formerly in the group of Ulrich Aschauer and moved to the chemical multinational company Dow.
- **Elsa Passaro**, formerly with Nicola Marzari's group and then senior software quality engineer at the open-source software company RedHat.
- **Daniel McNally**, a member of Thorsten Schmitt's group in phase I and then in the publishing industry as a senior editor at *Nature Materials*.

KTT: 200+ ACTIVITIES ORGANIZED OR SPONSORED

<https://nccr-marvel.ch/outreach/knowledge-transfer/activities-organized-sponsored-by-marvel>

- International symposium and workshop “Electronic Structure Theory for the Accelerated Design of Structural Materials”, Moscow, October 26-30, 2015.
- CECAM school “4th CP2K Tutorial”, CECAM-ETHZ, Zurich, August 31 to September 4, 2015.
- CECAM workshop “Future Technologies in Automated Atomistic Simulations”, CECAM-HQ-EPFL, Lausanne, June 8-10, 2015.
- International conference “Nothing is Perfect — The Quantum Mechanics of Defects”, Ascona, April 26-29, 2015.
- AiiDA workshop, Berlin, February 5, 2015.
- “Khartoum Workshop for the Advancements in Material Sciences” (KWAMS-15), Khartoum, February 1-10, 2015.
- CECAM conference “Frontiers of first- principles simulations: materials design and discovery”, Berlin, February 1-5, 2015.

[...]

[...]

- Quantum Computing Hard- and Software summer school, June 15-18, 2021.
- ETHZ/EPFL Summer School "Big Data and Machine Learning in Chemistry", EPFL (online), June 7-9, 2021.
- AiiDA tutorial at the MaX School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO, online, May 28, 2021.
- MRS Spring meeting 2021, Symposium NM04 "Magnetic Skyrmions and Topological Effects in Materials and Nanostructures", online, April 21, 2021.
- AiiDA tutorial at the Federal University of ABC, São Paulo, Brazil, February 10, 2021.
- Winter School on Density functional practice, online, February 1, 2021.
- MOLSIM2021 winter school, Amsterdam, Netherlands (online), January 4-15, 2021.

[...]

[...]

- CECAM workshop "Uncertainty quantification in atomistic modeling: From uncertainty-aware density functional theory to machine learning", Lausanne, Switzerland, November 25-28, 2025.
- Basics of software development workshop, Brisbane, Australia, November 11, 2025.
- Hubbard Workshop 2025 "The determination of Hubbard parameters: progress, pitfalls, and prospects", Gandia, Spain, September 22-26, 2025.
- CECAM workshop "Open Databases Integration for Materials Design (OPTIMADE)", Vilnius, Lithuania, September 15-19, 2025.

[...]



EO: MARVEL INSPIRE FELLOWSHIPS

INSPIRE Potentials: launched in 2016, 62 fellows were supported for Master's projects in 24 MARVEL groups across 8 institutions; 20 continued at PhD level in current or former MARVEL groups, 24+ elsewhere



November 2025 call

- **Lisa Ruth Andreozzi** (Sapienza Università di Roma, Italy) in the Marzari group at EPFL
1st March 2026 – 31 August 2026
- **Natalie E. Hooven** (University of Wisconsin, Madison, USA) in the Ceriotti group at EPFL
1st May 2026 – 31 October 2026
- **Ruth Mora Soto** (Universitat Politècnica de Catalunya, Spain) in the Holmes group at EPFL
1st July 2026 – 30 September 2026

April 2025 call

- **Veronika Lamparská** (University of Stuttgart, Germany) in the Carleo group at EPFL
15 September 2025 – 15 March 2026
- **Sofia Petrucci** (KU Leuven, Belgium) in the Cominboeuf group at EPFL
1st December 2025 – 31 May 2026
- **Mridula Venkatarayanan** (EPFL, CH) in the Tavernelli group at IBM
1st January 2026 – 30 April 2026

October 2024 call

- **Maria Andolfatto** (Università Milano-Bicocca, Italy) in the Marzari group at EPFL (anticipated evaluation)
1st November 2024 – 30 April 2025
- **Cecilia Botta** (Università degli Studi di Trieste, Italy) in the Passerone group at Empa
1st March 2025 – 31 October 2025
- **Sofia Chorma** (ENSTA, France) in the Ceriotti group at EPFL
1st April 2025 – 30 September 2025
- **Niya Petkova** (University of St Andrews, UK) in the Carleo group at EPFL
1st January 2025 – 31 January 2026

April 2024 call

- **Sofia Chorma** (ENSTA, France) in the Ceriotti group at EPFL (anticipated evaluation), summer internship
13 May 2024 – September 2024
- **Katja Moos** (Unifr, CH) in the Schuler group at Unifr
1st January 2025 – 30 June 2025

October 2023 call

- **Serena Bragadini** (UNIMORE, Italy) in the Marzari group at EPFL
1st March 2024 – 31 October 2024
- **Valentina Sanello** (Univ. Milano-Bicocca, Italy) in the Marzari group at EPFL
1st April 2024 – 30 September 2024
- **Hela Mhiri** (ENIT, Tunisia and ENSTA, France) in the Holmes group at EPFL
15 April 2024 – 14 December 2024
- **Jayashree Narayan** (IISER Mohali, India) in the Bonella group at EPFL
26 August 2024 – 25 February 2025

April 2023 call

- **Jente Clarysse** (ETHZ, CH) in the Luisier group at ETHZ
24 April 2023 – 23 October 2023
- **Anna Paulish** (EPFL, CH) in the Marzari group at EPFL
1st August 2023 – 31 January 2024
- **Ayesha Ulde** (IITM, India) the Raju Hatarajan group at EPFL
1st February 2024 – 15 February 2024
- **Aude Maier** (EPFL, CH) in the Zdeborová group at EPFL
1st October 2023 – 31 March 2024
- **Laura Mismetti** (EPFL, CH) in the Tavernelli group at IBM
18 September 2023 – 11 March 2024

October 2022 call

- **Linda Mauren** (EPFL, CH) in the Carleo group at EPFL
1st January 2023 – 30 June 2023
- **Noémie Xiao Hu** (EPFL, CH) in the Smit group at EPFL
27 February 2023 – 26 August 2023
- **Melika Honarmand** (Tehran Polytechnic, Iran) in the Ceriotti group at EPFL
15 January 2023 – 14 July 2023
- **Eva Dolazekski** (TU Wien, Austria) in the Rimiker group at ETHZ
18 September 2023 – 17 March 2024

April 2022 call

- **Arianna Cantarella** (University of Parma, Italy) in the Pizzi group at EPFL
1st October 2022 – 31 March 2023

October 2021 call

- **Virginie de Mestral** (EPFL, CH) in the Luisier group at ETH Zurich
1st October 2021 – 31 March 2022
- **Nataliya Paulish** (EPFL, CH) in the Marzari group at EPFL
15 September 2022 – 15 March 2023
- **Mie Engelbrecht Jensen** (DTU, Lyngby, Denmark) in the Spaldin group at ETHZ
21 February 2022 – 20 August 2022

April 2021 call

- **Nanchen Dongfang** (University of Zurich, CH) in the Hutter group at UZH
1st July 2021 – 31 December 2021
- **Emma Lumiaro** (Aalto University, Finland) in the Ceriotti group at EPFL
15 September 2021 – 15 March 2022
- **Mathilde Franckel** (Ecole Européenne de Chimie, Polymères et Matériaux de Strasbourg, France) in the Pasquarello group at EPFL
15 February 2022 – 15 August 2022

October 2020 call

- **Elena Gazzarini** (King's College London, UK) in the Marzari group at EPFL
15 January 2021 – 14 July 2021
- **Yuri Cho** (University of Basel, CH) in the von Lilienfeld group at UniBas
1st March 2021 – 31 August 2021

April 2020 call

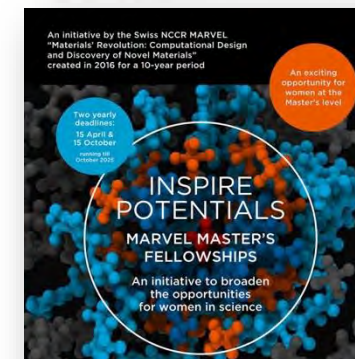
- **Veronica Michel** (ETH, Zurich, CH) in the Spaldin group at ETHZ
18 May 2020 – 5 October 2020
- **Miriam Stuke** (University of Basel, CH) in the von Lilienfeld group at UniBas
10 August 2020 to 9 February 2021
- **Maria Pakhnova** (Moscow Institute of Physics and Technology (MIPT), Russia) in the Ceriotti group at EPFL
1st November 2020 to 30 April 2021

October 2019 call

- **Dune André** (Ecole Normale Supérieure, Paris, France) in the Cominboeuf group at EPFL
19 February 2020 – 19 August 2020
- **Yuting Chen** (ETH, Zurich, CH) in the Passerone group at Empa
1st March 2020 – 31 August 2020

April 2019 call

- **Jigyasa Nigam** (Indian Institute of Space Science and Technology (IIST), Trivandrum, Kerala, India) in the Ceriotti group at EPFL
15 August 2019 – 15 February 2020
- **Joanna Stoycheva** (Sofia University "St. Kliment Ohridski", Bulgaria) in the Ceriotti group at ETHZ
1st November 2019 – 30 April 2020
- **Linnea March Folkmann** (University of Copenhagen, Denmark) in the Ceriotti group at EPFL
1st November 2019 – 30 April 2020



October 2018 call

- **Tara Niamh Tósić** (EPFL, CH) in the Spaldin group at ETHZ
1st March – 31 August 2019
- **Julietta Trapé** (National University of Cuyo, Mendoza, AR) in the Parrinello group at USI
1st June – 30 Nov 2019
- **Sinjini Bhattacharjee** (Indian Institute of Science Education and Research (IISER), Pune, IN) in the Cominboeuf group at EPFL
15 May – 15 Nov 2019
- **Maria Syzgantseva** (Lomonosov Moscow State University, RU) in the Smit group at EPFL
15 April – 15 October 2019
- **Chiara Devescovi** (Sacred Heart Catholic University, Brescia, IT) in the Soluyanov group at UZH
1st May – 31 October 2019

April 2018 call

- **Charlotte Müller** (University of Zurich, CH) in the Hutter group at UZH
1st October 2018 – 31 March 2019
- **Maria Bilichenko** (Oles Honchar Dnipro National University, UA) in the Hutter group at UZH
1st January – 30 June 2019

October 2017 call

- **Henglu Xu** (EPFL, CH) in the Smit group at EPFL
1st February – 31 July 2018
- **Rong Zhang** (Nanyang Technological University, Singapore) in the Marzari group at EPFL
15 February – 15 August 2018
- **Chiara Cignarella** (La Sapienza, Rome, IT) in the Hutter group at UZH
1st March – 31 August 2018
- **Martina Danese** (Università degli Studi di Trieste, IT) in the Passerone group at Empa
15 March – 15 September 2018
- **Melania D'Aniello** (La Sapienza, Rome, IT) in the Goedecker group at UniBas
15 August 2018 – 15 February 2019

April 2017 call

- **Andriani Keliri** (ETHZ, CH) in the Spaldin group at ETHZ
20 March – 25 September 2017
- **Özge Kadioğlu** (Koç University, Istanbul, TR) in the Smit group at EPFL
15 August 2017 – 31 January 2018
- **Nataliya Lepanitsyna** (Moscow Institute of Physics and Technology, RU) in the Ceriotti group at EPFL
1st October 2017 – 31 March 2018
- **Yuting Qian** (University of Chinese Academy of Science, Beijing, CN) in the Yazyev group at EPFL
15 October 2017 – 14 April 2018
- **Simran Kumari** (Indian Institute of Science Education and Research, Kolkata, IN) in the Marzari group at EPFL
1st December 2017 – 31 May 2018

October 2016 call

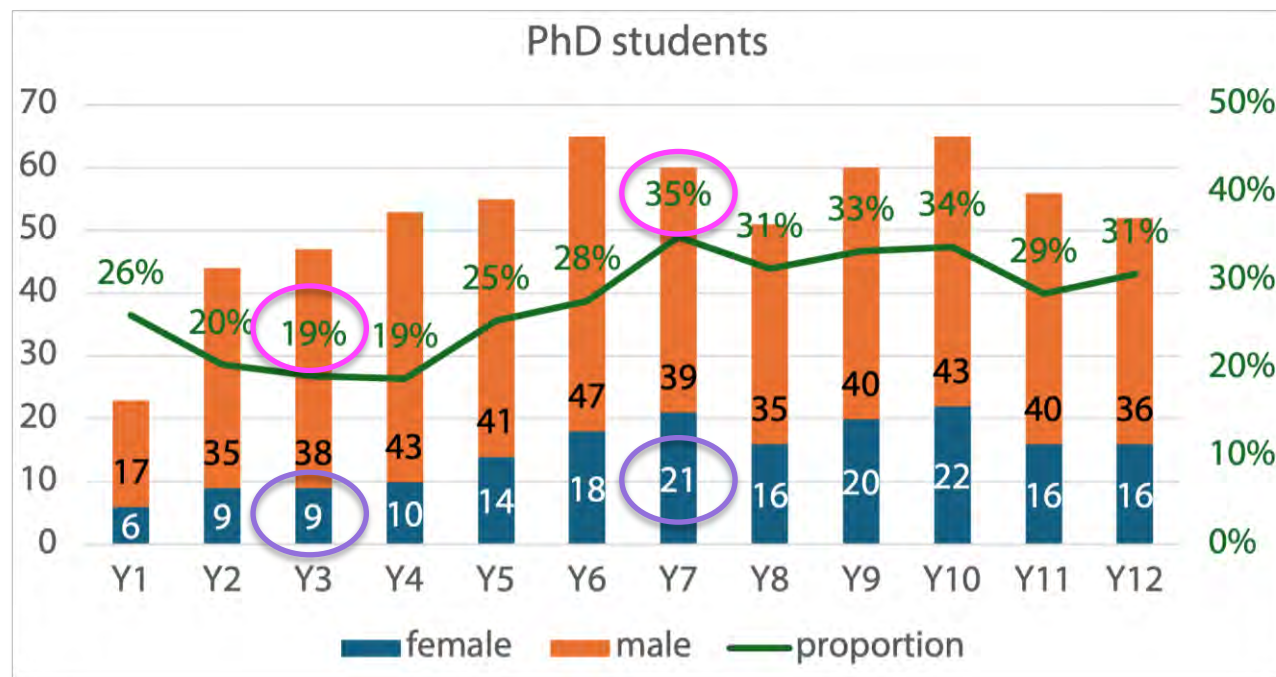
- **Alice Cuzzocrea** (Università degli Studi di Trieste, IT) in the Ceriotti group at EPFL
1st May – 31 October 2017
- **Cecilia Chiaracane** (Università degli Studi di Trieste, IT) in the Yazyev group at EPFL
1st May – 31 October 2017
- **Cecilia Vona** (Università degli Studi di Trieste, IT) in the Röthlisberger group at EPFL
1st May – 31 October 2017

May 2016 call

- **Norma Rivano** (Università degli Studi di Cagliari, IT) in the Marzari group at EPFL
1st March – 31 August 2017

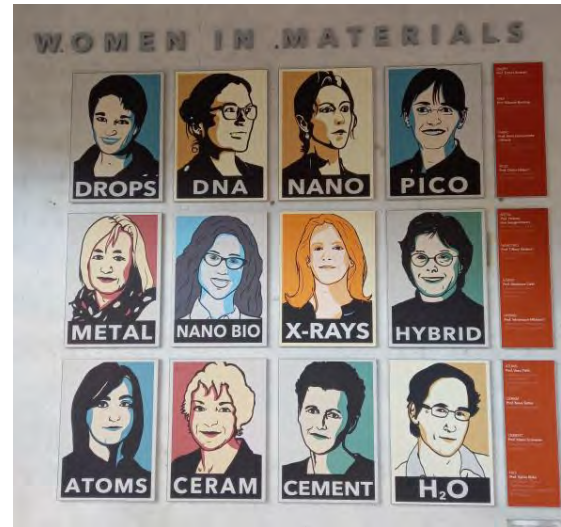
EO: INCREASING PhD RESEARCHERS

Doubling women PhD researchers: women represented **19%** of MARVEL PhD students in year 3, **35%** in year 7, and stabilized around **32%** in phase III; in absolute terms, the number of women PhD students more than doubled from **9 to 21** between year 3 and year 7.



EO: VISIBLE ROLE MODELS

From fellowship scheme to culture change: Agility Plus funding for women PIs, gender-bias and leadership workshops, outreach for girls, #NCCRWomen, public portraits/interviews, and long-term through EPFL's MX Master fellowship and continuing outreach activities.




#NCCRWomen
Women in Swiss Research



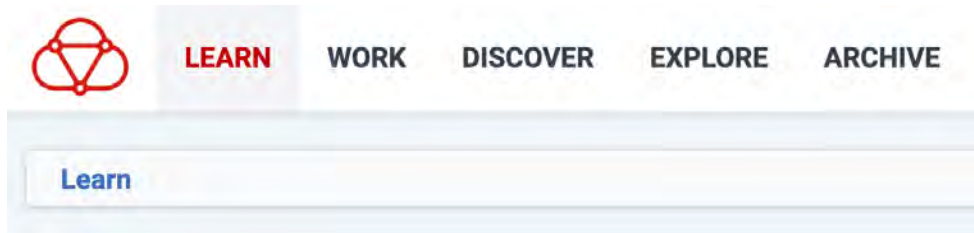
ET: JUNIOR RETREATS AND JUNIOR SEMINARS

Junior researchers as organizers: junior retreats and seminars trained leadership, communication and collaboration. **6 junior retreats gathered 50-60 young researchers that self-organized** and generated project ideas across institutions. **Junior seminars were held monthly**, and will continue post-MARVEL.

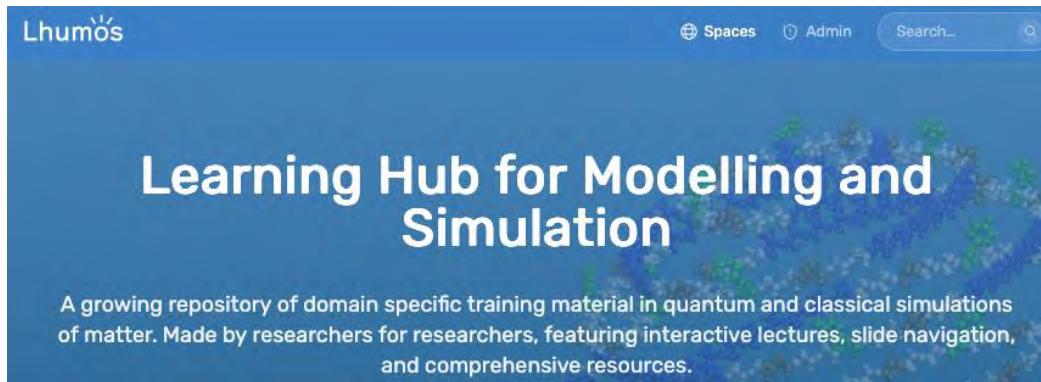


ET: DIGITAL EDUCATION

Digital education: Learn, Lhumos, Quantum Mobile, OSSCAR. Materials Cloud Learn and Lhumos preserved lectures and tutorials; Quantum Mobile and OSSCAR lowered the entry barrier for computational materials teaching. Materials Cloud Learn averaged about **500 unique visitors per month** from fall 2020 onward.



www.materialscloud.org/learn



lhumos.org



Open Software Services for Classrooms and Research

www.ossicar.org



quantum-mobile.readthedocs.io



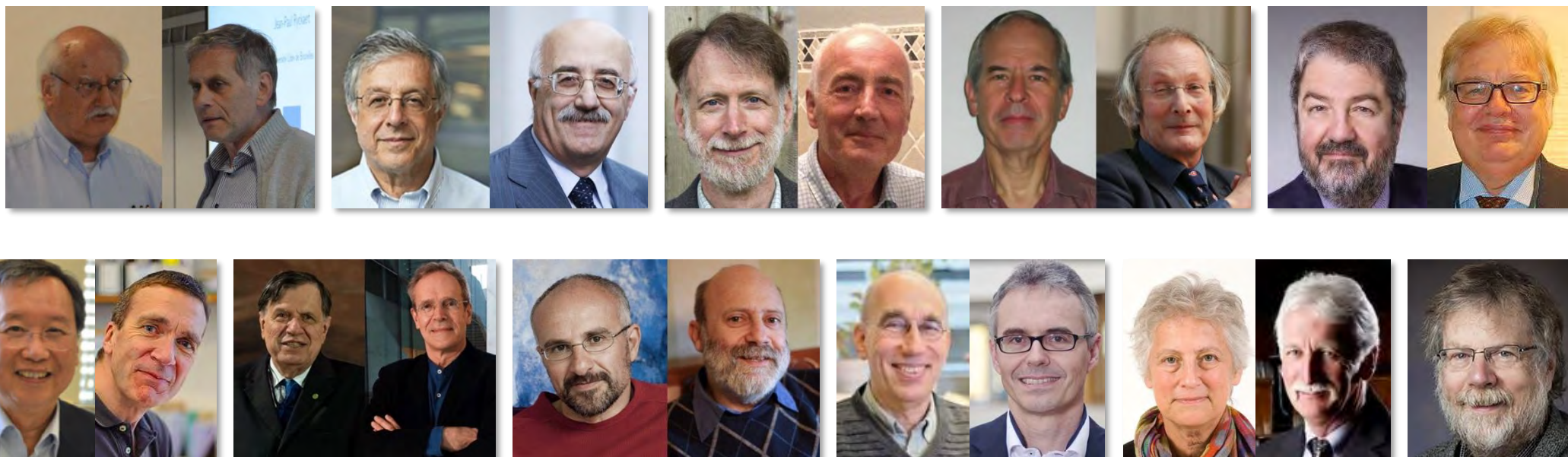
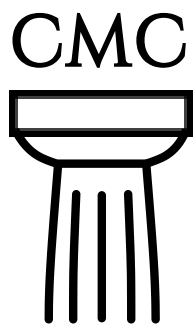
ET: 41 MARVEL DISTINGUISHED LECTURES

International training footprint: 41 MARVEL Distinguished Lectures – during CoVid we reached the record of 700+ participants for Georg Kresse. All recorded on MC Learn and Lhumos.



ET: CECAM-MARVEL CLASSICS

International training footprint: 11 CECAM-MARVEL Classics – alternating statistical mechanics and electronic-structure theory (for the latter, from Car-Parrinello to the modern theory of polarization, from GW to dynamical mean field theory, TDDFT, and QMC).



ET: MARY-ANN MANSIGH CONVERSATIONS

International training footprint: 7 CECAM-MARVEL Mary Ann Mansigh Conversations
From MAM herself to Olivetti 101, from diplomacy to cancel culture, passing through
Industry and scientific writing



ET: MARY-ANN MANSIGH CONVERSATIONS

International training footprint: 7 CECAM-MARVEL Mary Ann Mansigh Conversations
From MAM herself to Olivetti 101, from diplomacy to cancel culture, passing through
Industry and scientific writing



ET: TRAINING FOOTPRINT – HIGH-SCHOOL CAMPS



ET: TRAINING FOOTPRINT – ASESMA ET AL

International training footprint: deep engagement with ASESMA, African MRS, EXAF, and the creation of ASESMAnet.



ET: ICTP-MARVEL COLLEGE ON MATERIALS SIMULATIONS IN THE AGE OF AI

228 participants, 57 nationalities (this latter was ICTP record!); thanks to MARVEL, 66 full fellowships, 99 partial fellowships.



CO: 170+ SCIENCE HIGHLIGHTS, 260 NEWS ITEMS, 61 PRESS RELEASES

A professional editorial channel for computational materials science: The MARVEL website evolved from a project page into a communication platform: by 2026 it hosted **170+ science highlights or feature stories**, **260+ news items**, and MARVEL had issued **61 press releases** through EurekAlert since 2019.



X account (2200 followers)

Enhances MARVEL visibility, helps spread research and news more widely.



LinkedIn account (880+ followers)

Private group (NCCR MARVEL Members and Alumni): 135 members



CO: Ig NOBEL AWARD TOUR; OPEN DAYS/SCIENTASTICS

Public outreach: The Ig Nobel Award Tour Show became a signature event with 500-700 attendees;
Open Days, Scientastic, school visits, 3D movies and hands-on demonstrations translated topics such as 2D materials, phonons, magnons and materials landscapes for broad audiences.



CO: Psi-k 2022, Psi-k 2025 – 1300+ IN-PERSON PARTICIPANTS

Global visibility through Psi-k: Psi-k 2022 and Psi-k 2025 positioned EPFL/Switzerland as a central hub for first-principles materials simulations; each had **1,300+ in-person participants**.



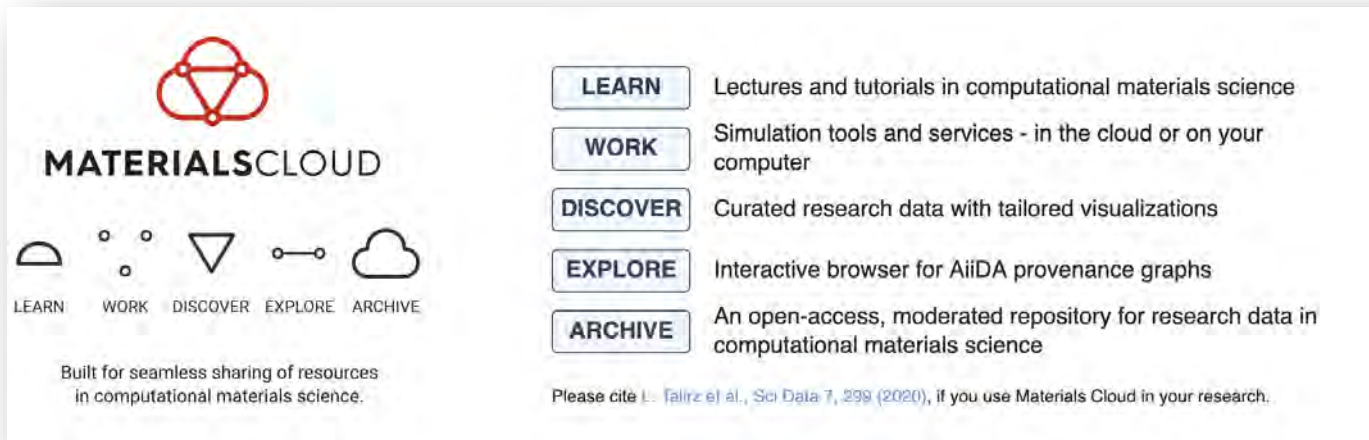
<https://www.psik2022.net/>

<https://www.psik2025.net/>



OPEN SCIENCE

From FAIR data to FAIR simulations: MARVEL did not just ask people to upload data; it built an ecosystem —Materials Cloud, AiiDA/AiiDALab, Quantum Mobile, Materials Cloud Learn, Lhumos and OSSCAR — **to make simulations reproducible, shareable, teachable and reusable**



OPEN SCIENCE

Materials Cloud Archive as a recognized repository: The Archive reached its 1,000th record on 3 April 2024 and is recommended by the European Commission, SNSF and *Nature Scientific Data*.

Number of published records (all versions): 1485 Number of published records (latest version): 1208

Latest records

Number of published records (all versions): 1485
Number of published records (latest version): 1208
This page shows the latest version of each record.

Twinned-magnesium metal anodes enable reversible magnesium electrodeposition
DOI: 10.26434/chemrxiv-2024-1p1y1
Zou, Guodong; Ren, Jingli; Wang, Jinming; and 7 others
The favourable thermodynamic properties of magnesium (Mg) make it a promising anode for rechargeable Mg-metal batteries. However, parasitic side reactions and uncontrolled deposition at the unstable electrode/electrolyte interface severely hinder reversible electrodeposition. Here we demonstrate that a high density of twin defects via cyclic-mul...
Latest version: v1
Publication date: July 3, 2026

In search of novel ductile superconductors
DOI: 10.26434/chemrxiv-2024-1p1y1
Zhang, Yiming; Poncè, Samuel
We perform a first-principles high-throughput screening of the mechanical properties of phonon-mediated superconductors derived from the recent experimentally synthesized superconducting materials database PRX Energy 4(4), 033012 (2025). We develop the aiida-mechanical workflow which combines first-principles calculations of elastic constants...
Latest version: v1
Publication date: July 3, 2026

Exceptionally high carrier mobility in hexagonal diamond
DOI: 10.26434/chemrxiv-2024-1p1y1
Ho, Zirui; Gao, Shang-Peng; Chen, Meng
This dataset supports the theoretical investigation reported in the manuscript "Exceptionally high carrier mobility in hexagonal diamond". Based on first-principles analyses of the electronic structures, carrier mobilities, and electron-phonon coupling mechanisms in both cubic diamond and hexagonal diamond, this work demonstrates high carrier mobility...
Latest version: v1
Publication date: July 1, 2026

Connected applications and tools

Browse records linked to these applications and tools

- Materials Cloud
Discover/Explore/Tools
- Optimade
- Chemiscope
- AiIDA + Renku

The Materials Cloud Archive has published its 1000th record

This was published on April 3, 2024

Launched in 2017, this open repository for materials science data has kept growing constantly since then and is now one of the repositories of choice recommended by the European Commission, the Swiss National Science Foundation and *Nature Scientific Data*. A new version with improved features will be launched in the second half of 2024, while the BIG-MAP project will apply the same technology to create a restricted-access archive for sharing data within collaborations.

by Nicola Niseng, NCCR MARVEL

Seven years after receiving its very first submission, the **Materials Cloud Archive** has reached an important milestone on 3 April with the publication of the 1000th record. Titled "Phonon-limited mobility for electrons and holes in highly-strained silicon", the latest addition to the Archive contains data based on first-principles calculations to explore the variations of the mobility of electrons and holes in silicon upon deformation by uniaxial strain, and comes from Samuel Poncè's group at the Université catholique de Louvain in Belgium.

Launched in 2017, this open repository for materials science data has kept growing constantly since then and is now one of the repositories of choice recommended by the **European Commission**, the **Swiss National Science Foundation** and **Nature Scientific Data**.

The Materials Cloud Archive offers scientists the possibility to upload data connected to a research article, in a format that facilitates the reuse of data by other researchers. The Archive itself and datasets published on it are indexed by top registries such as [re3data](#), [fairsharing.org](#), [Google Dataset Search](#) and [Eudat's B2FIND](#).

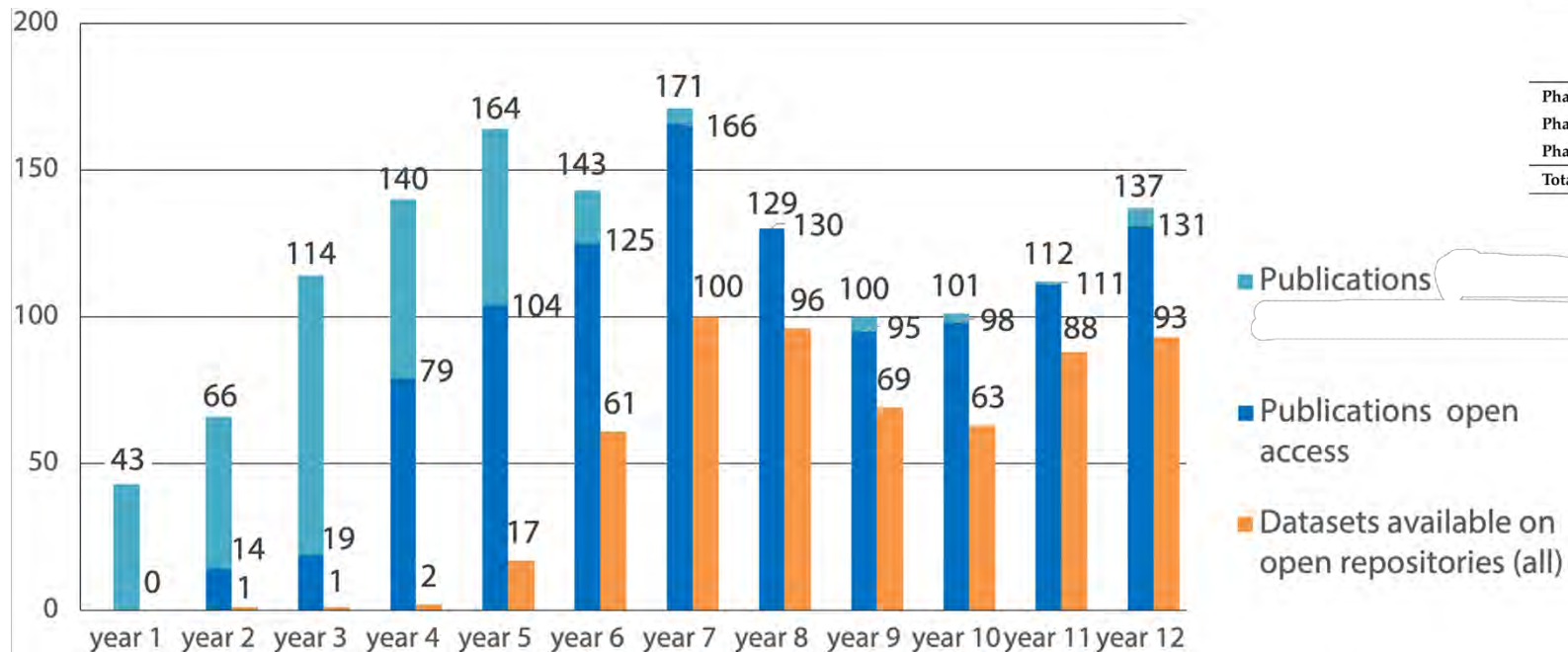
Records published (URL assigned)

Materials Cloud Archive: number of records published per year.



OPEN SCIENCE

Open-access culture and dataset discipline: MARVEL went from **31% open-access publications in phase I** to **86% in phase II** and **97% in phase III**, **with 1,420 publications and roughly 600 datasets indexed or deposited**, mainly through Materials Cloud.



	All publications					Datasets	
	Research articles in science journals	Review article	Book / Contribution to a book	Proceedings	Editors / Other	Total	Datasets (on FAIR data repositories)
Phase I	352 (97%)	2	4	5		363	7
Phase II	556 (92%)	23	17	11		607	271
Phase III	419 (93%)	20	1	9	1	450	314
Total	1'327 (93%)	45	22	25	1	1'420	592

OPEN  ACCESS

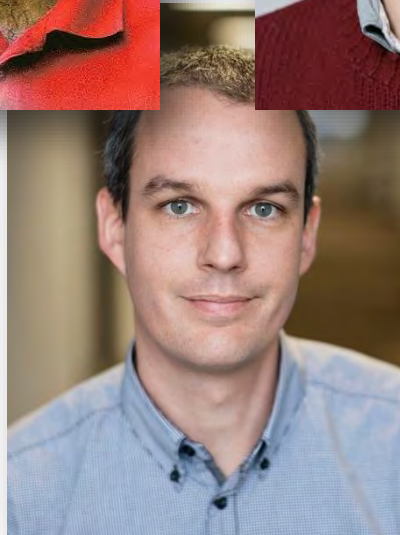


MATERIALSCLOUD



ERC GRANTS

Internationally visible leaders: 27 ERC grants (24 EU + 3 SNSF “ERC replace”)



ERC Grants

The following 24 ERC Grants and 3 SNSF ERC “replacement” Grants have supported MARVEL members during or after their participation in the Centre.

Started 2025

- **Statistical Physics of Attention and Sequence Modelling with Neural Networks (SPASM-net)**, *Advanced Grant*, Lenka Zdeborová, 2025-2029.

Started 2024

- **Interacting topological quantum chemistry**, *SNSF Consolidator Grant*, Titus Neupert, 2024-2028.

Started 2023

- **Big Data in Nanoporous Materials: Science beyond Understanding**, *SNSF Advanced Grant*, Berend Smit, 2023-2028.

Started 2022

- **Quantum Transport Simulations at the Exascale and Beyond (QuaTrEx)**, *SNSF Advanced Grant*, Mathieu Luisier, 2022-2027. [More information](#)
- **Fiamma** (Fully Integrating Atomistic Modeling with Machine Learning), *Consolidator*, Michele Ceriotti, 2022-2026. [More information](#)

Started 2019

- **PushQChem** (Pushing Quantum Chemistry by Advancing Photoswitchable Catalysis), *Consolidator*, Clémence Corminboeuf, 2019-2024. [More information](#)
- **HERO** (Hidden, entangled and resonating orders), *Synergy*, Nicola Spaldin, Gabriel Aeppli, Henrik Rønnow and Alexander Balatsky, 2019-2025. [More information](#)

Started 2018

- **QML** (Quantum Machine Learning: Chemical Reactions with Unprecedented Speed and Accuracy), *Consolidator*, Anatole von Lilienfeld, 2018-2023. [More information](#)
- **PARATOP** (New paradigms for correlated quantum matter: Hierarchical topology, Kondo topological metals, and deep learning), *Starting*, Titus Neupert, 2018-2023

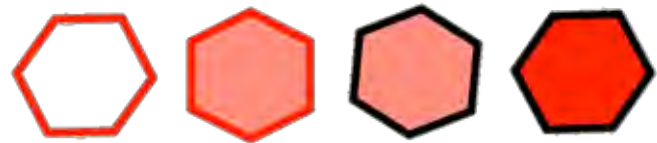
Started 2017

- **MODMAT** (Nonequilibrium dynamical mean-field theory: From models to materials), *Consolidator*, Philipp Werner, 2017-2022.
- **time-data** (Time-Data Trade-Offs in Resource-Constrained Information and Inference Systems), *Consolidator*, Volkan Cevher, 2017-2022.

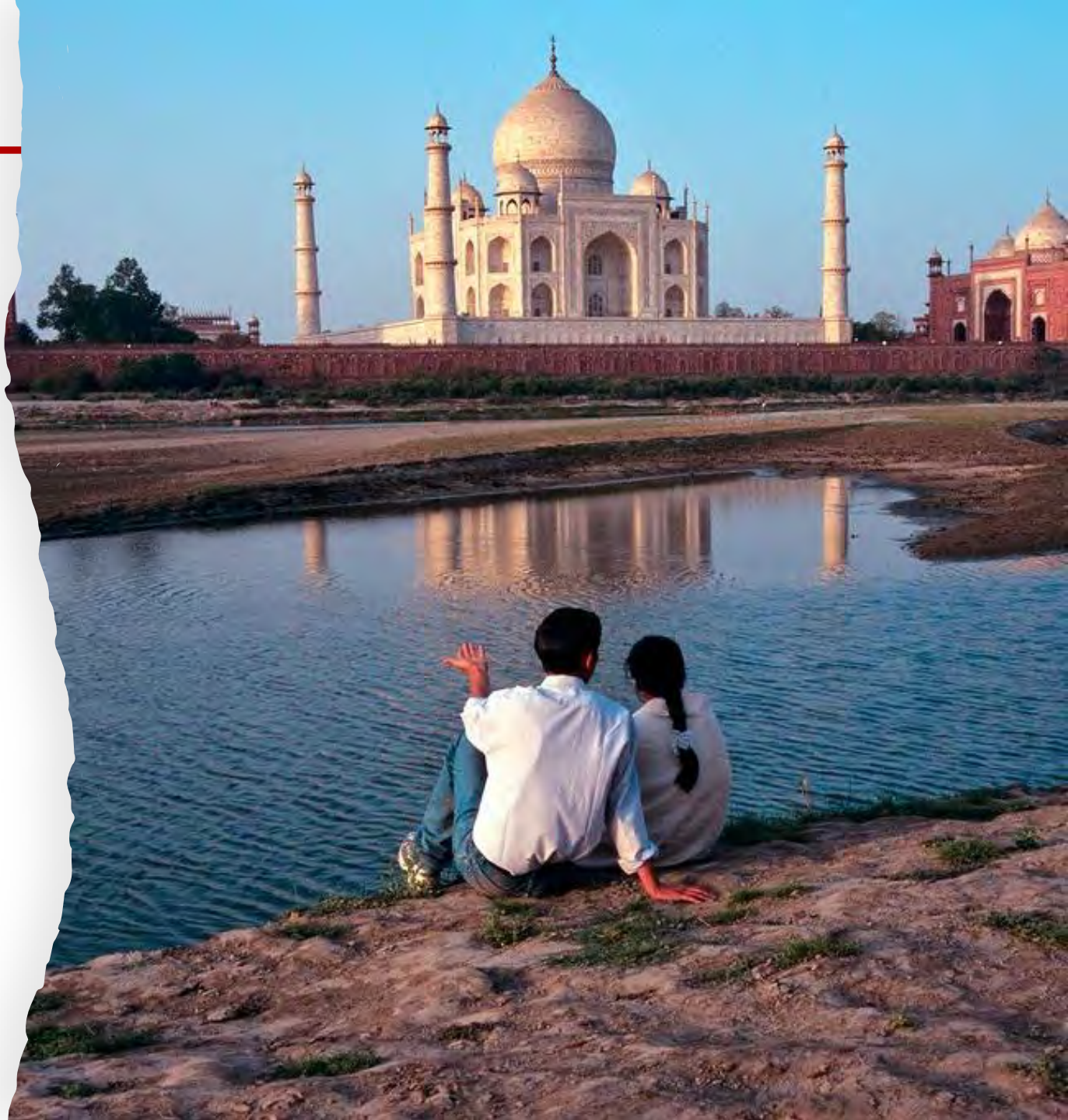


LEGACY AND UNDYING LOVE

MARVEL



NATIONAL CENTRE OF COMPETENCE IN RESEARCH



MAIN STRUCTURAL LEGACY

- **EPFL faculty renewal – 1 PATT in IMX, 1 PA/PO in IMX/PSI**
- **PSI Laboratory for Materials Simulations**
- **Materials Cloud & AiiDA/AiiDAlab**
- **CECAM and a Swiss CECAM node (CECAM-CH-MARVEL)**
- **Empa Scientific IT/AiiDAlab**
- **CSCS/SIRIUS**
- **Education/equal-opportunity continuation**

PSI Center of Scientific Computing, Theory and Data

Established in July 2021 – Now ~100 experts, 11 MCHF/y

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PSI Laboratory for Materials Simulations

LMS includes groups on Materials Software and Data (Pizzi), Multiscale Materials Simulations (Krack), and Light–Matter Interactions (Schueler), plus two tenure-track scientists (Colonna and Timrov).

Mission statement

- to develop, integrate, and disseminate in the PSI community and the scientific community at large the computational capabilities required to understand, predict, and characterize materials as studied at PSI research facilities with photons, neutrons, muons, and electrons.
- to provide support and access to these computational capabilities for the PSI science and user program.
- to curate the computational data for structures, properties, and spectra required to discover or design materials with novel or enhanced properties and performance.
- to perform own research at the forefront of computational materials simulations.

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UniFR-PSI joint appointment of Michael Schüler: light–matter interactions, tenure-track assistant professor and group leader in PSI Laboratory for Materials Simulations.

UniFR-PSI joint appointment of Dominik Juraschek: UniFR and PSI jointly hired Dominik Juraschek, in non-equilibrium quantum physics, as tenure-track assistant professor and group leader in PSI Laboratory for Theoretical and Computational Physics.

UniFR: The Faculty of Science and Medicine is inviting applications for the **position of Professor of Data-Driven Materials Discovery at the Adolphe Merkle Institute (AMI).**

- At Empa, AiiDAlab became a supported capability for different laboratories; the creation of a Scientific IT division at Empa as one of the major long-term deliverables.
- From Christian Leinenbach's additive-manufacturing group integrated into Pillar 1 to validate computational models through fabrication and testing, and AiiDA driving experiments on Empa's Aurora robotic platform

CSCS as the HPC/platform backbone

- Materials has become one of CSCS's two core communities/domains, including Materials Cloud Platform-as-a-Service
- SIRIUS and related workflows position MARVEL codes and workflows for future architectures, with LUMI/Alps-era scalability clearly showcased

Materials Cloud as a distributed long-term infrastructure

- Materials Cloud is the central international infrastructure legacy. Data storage and services are in place to support the platform at least until 2036, mostly at CSCS, with CECAM and CINECA Bologna taking over Archive services with additional personnel.
- By 2026, the AiiDA registry counted 106 plugin packages supporting 180 simulation codes and more than 200 workflows, many maintained outside MARVEL.
- Lhumos, Quantum Mobile, OSSCAR, Materials Cloud Learn and recorded lectures convert training into durable learning infrastructure.

EU embedding: MaX, Materials Commons, MatOSC/EOSC

- MARVEL's digital infrastructure has become part of broader European materials-modelling infrastructure.
- MaX (Materials Design at the eXascale, 2015-onwards, just renewed for 2027-29).
- Materials Commons (2026-2029)
- MatOSC – preparatory phase

Research-data-management culture and FAIR simulations

- MARVEL moved from open data to the idea of FAIR simulations, with a data team, RDM strategy, DOI-based repositories, versioning, long-term preservation, and a funded storage/sharing infrastructure.
- 1,420 publications, 600 datasets in the dataset index, and 40+ open codes, from major to focused

A distributed national legacy model

- EPFL remains the main academic home; PSI provides the explicit long-term laboratory/divisional framework; Empa provides complementary experimental/computational embedding; CSCS remains the HPC and platform backbone.