MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Materials' Revolution: Computational Design and Discovery of Novel Materials

Final Report

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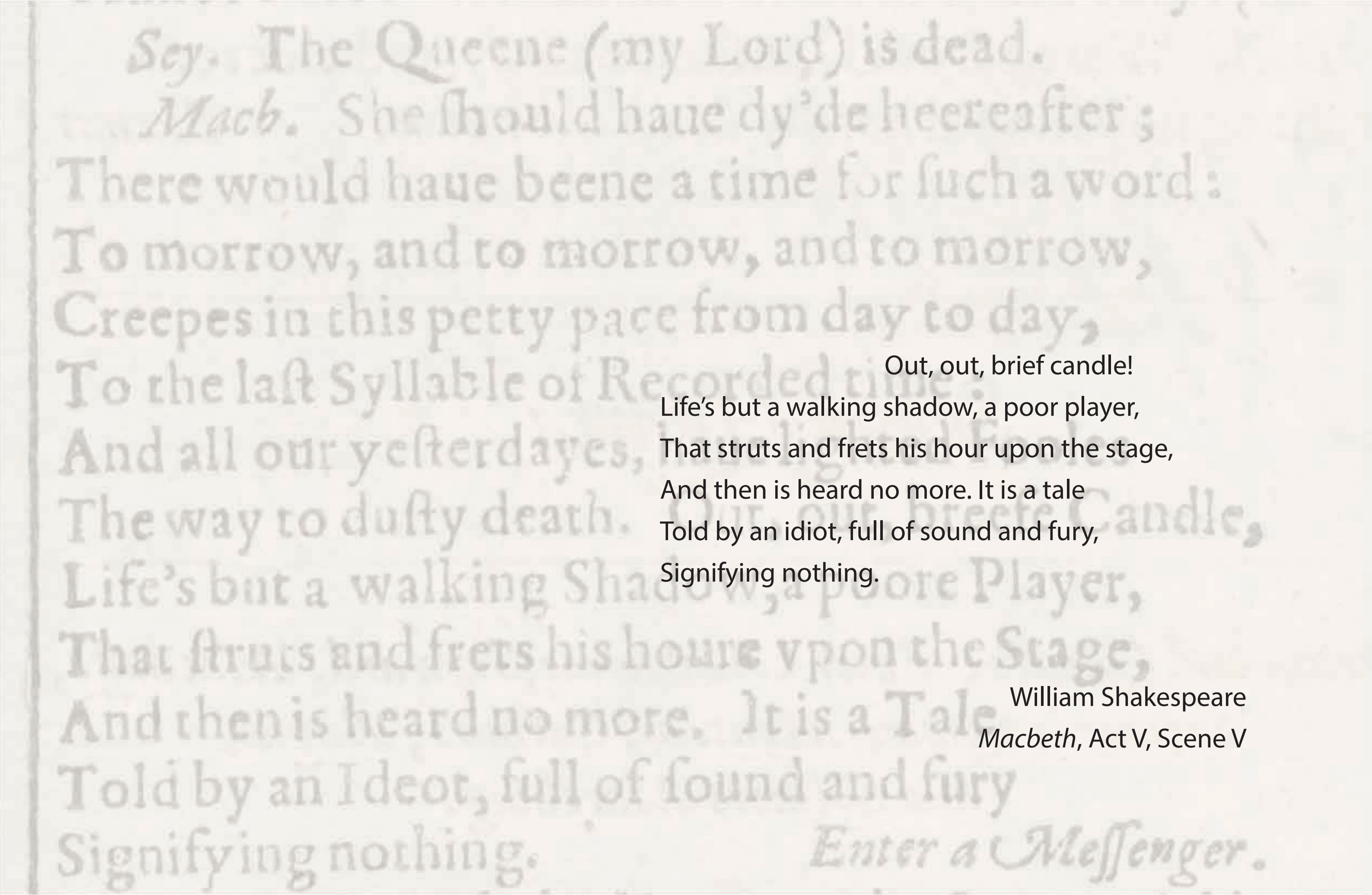

Sey. The Queene (my Lord) is dead.
Macb. She ſhould haue dy'de heereafter;
There would haue beene a time for ſuch a word:
To morrow, and to morrow, and to morrow,
Creepes in this petty pace from day to day,
To the laſt Syllable of Recorded time:
And all our yeſterdayes, haue lighted Fooles
The way to duſty death. Out, out, breefe Candle,
Life's but a walking Shadow, a poore Player,
That ſtruts and frets his houre vpon the Stage,
And then is heard no more. It is a Tale
Told by an Ideot, full of ſound and fury
Signifying nothing. *Enter a Meſſenger.*

Out, out, brief candle!
Life's but a walking shadow, a poor player,
That struts and frets his hour upon the stage,
And then is heard no more. It is a tale
Told by an idiot, full of sound and fury,
Signifying nothing.

William Shakespeare
Macbeth, Act V, Scene V

Swiss National
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NCCR series 4 Final Report – cover sheet, template & explanations

Title of the NCCR	Materials' Revolution: Computational Design and Discovery of Novel Materials (MARVEL)
NCCR Director(s) / Co-Director(s)	Marzari Nicola, EPFL, 01/05/2014 – 31/07/2026
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9. Feedback and concluding remarks of the NCCR director(s)

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1 Executive summary

It is worthwhile to go back to where we started — reporting here verbatim the original MARVEL plan, as submitted in the 2012 preproposal:

Summary: *Accelerated design and discovery of materials displaying novel physics or improved properties, via a materials' informatics platform of database-driven, high-throughput quantum simulations whose predictive accuracy is supported by advanced or innovative electronic-structure capabilities, is verified and validated thanks to code interoperability and automated benchmarking, and is applied to materials for energy, information-and-communication technologies, and pharmaceuticals. The goal of this proposal is to radically transform and accelerate invention and discovery in science and technology, and especially to transform and accelerate the design and discovery of novel materials in order to achieve improved properties and performance, or to witness the emergence of original physical properties. We will achieve this goal by exploiting the predictive accuracy that quantum-mechanical simulations have now reached for realistic, complex systems, the treasure trove of ever-increasing computational power ideally suited to intrinsically parallel problems, and the powerful synergies arising from the computer science of heterogeneous data management, data mining, and machine learning.*

By combining accurate, realistic, and predictive simulations of materials with an infrastructure able to run or interrogate thousands to hundreds of thousands calculations at a time we will be able to explore phases, structures, and compositions in materials' space searching for the emergence of novel and fundamental physical properties or for the optimal combination of, e.g., performance, price, and durability, in the quest for better, cheaper, or more environmentally sound materials. We will thus develop a layer of materials' informatics where we can run queries in a database-driven mode, where we provide a natural platform to move the field of quantum simulations from the narrower picture of case-by-case explorations to a broader vista of questions posed for entire classes of materials, where we can rapidly respond to the discovery of novel classes of materials or of physical properties, and where data mining and machine learning complement our established approaches based on intuition and intelligence. Much needed verification and validation will be achieved by code interoperability and by extensive benchmarking against experimental results. We will apply this research platform to key strategic areas for societal development and well-being, where improved materials translate directly into improved performance: from the harvesting, storage, and conversion of energy, to information and communication technologies, to pharmaceuticals, with deliverables that will focus on novel multifunctional materials (multiferroics, light harvesters, superconductors, magnets, topological materials), novel materials for energy applications (batteries, photovoltaics, solar fuels, thermoelectrics), and organic molecular crystals.

Our ultimate, long-term goal is an infrastructure able to simulate and discover or invent materials and devices with an accuracy often comparable or even exceeding that of experiments, and with a speed that mirrors the speed at which computation, data storage, and processing improve, rather than mirroring the constraints of our physical laboratories, manpower, and creativity.

Also, in the same 2012 preproposal, the materials informatics infrastructure is presented:

The materials informatics infrastructure will be composed by:

the writers: *a community of database-driven interoperable quantum engines (*QUANTUM ESPRESSO, *Abinit*, CP2K*);*

the library: *a database of materials, of materials' properties and performance, and of the results of quantum simulations, that starts with the structures of known materials, and that continuously expands, with the writers computing the missing pieces that represent the vast majority of the database: materials still undiscovered but stable or metastable, properties not yet measured, and architectures not yet assembled;*

the language: *a data management system that allows to store data heterogeneously, in its original and usually most natural format, while still providing the ability to uniformly and effi-*

ciently access, query, and analyze it, and a single unified language for accessing all the data known to the system in a format that allows the easy expression of materials science terminology;

the librarian: *the agent that controls the quantum engines, reads the library, directs the effort to fill the library with the missing pieces, and addresses the grand challenges of the vertical materials design projects.*

This vision seems as fresh and compelling now as it was 14 years ago: some of the giant internet companies — from Google/Deepmind to Microsoft to Meta — have started in the past 2-3 years major efforts in materials design and discovery, and this is mirrored by an influx of startups in the field (such as CuspAI, Lila Sciences, Periodic Labs, and Radical AI), raising more than 800 million dollars at first entry. And agentic AI has now become a reality.

The overall summary is that MARVEL had and still has exactly the right mission, drive, and ambition; at the same time, the need to fulfill multiple tasks and strategies, engage multiple stakeholders, and keep an otherwise well funded Swiss community focused on the goals of the project meant that the human resources were often stretched thin. It certainly showed, like many efforts worldwide, that materials can be discovered faster when theory, algorithms, high-performance computing, data, machine learning and experiments are tightly connected. Importantly, it kept pushing an agenda of open-source codes, open-access data, and of much needed verification efforts — often remarkably missing in a field that produces tens of thousands of papers per year. It produced new scientific knowledge, built digital tools used far beyond the consortium, trained a new generation of researchers, widened participation, and created lasting structures that strengthen Switzerland's position in computational materials science.

Research: advances in electronic-structure theory and methods, and their application to materials discovery — from quantum materials to energy materials, molecular materials, and advanced alloys.

Structure: a national network linking EPFL, ETH Zurich, PSI, Empa, CSCS and Swiss universities, with durable post-NCCR hubs.

Open science: AiiDA/AiiDAlab and Materials Cloud made workflows, data and teaching materials openly reusable; Materials Cloud passed 1'000 *Archive* records in 2024.

Knowledge and technology transfer: MARVEL built ties with dozens of companies, 17 in phase III, and over the 12 years company-linked projects involved almost CHF 7 millions in funding.

Equal opportunities: 62 INSPIRE Potentials fellows were supported; the number of women PhD researchers in the NCCR doubled during phase II.

Education and training: schools, tutorials, seminars and camps trained learners from high-school level to postdoctoral level; 41 Distinguished Lectures, 11 CECAM-MARVEL Classics, 7 CECAM-MARVEL Mary-Ann Mansigh Conversations.

Communication & outreach: a professional website, regular newsletters, feature stories and science highlights, press releases, social media and public events.

This, combined with the long-term strategic collaboration with CECAM, the close involvement with Psi-k and the organization in 2022 and 2025 of the two general Psi-k conferences (1'300+ in-person participants in both cases), and the myriad educational activities meant that the visibility and leadership of MARVEL has been very apparent worldwide.

A faster way to discover materials

MARVEL's central achievement was to make materials discovery more predictive, more systematic and more collaborative. Instead of relying mainly on trial and error in the laboratory, the NCCR combined physics, chemistry, computer science, high-performance computing and experiments to identify promising materials earlier, understand why they work, and share the underlying methods with others.

On the scientific side, MARVEL produced important results in several areas. It kept developing **advanced electronic-structure methods**, able to treat excitations and correlations with predictive accuracy, while also improving the descriptions of materials in the ground state, and incorporating many of these capabilities in open-source codes, or laying the foundations for perturbative approaches. It pioneered **machine-learning methods for molecules and materials**, developing novel foundational models that represent the state-of-the-art in the field. It pushed **core verification efforts** — from protocols for reliable simulations to major verification efforts of pseudopotentials against all-electron data.

It predicted and helped confirm new **quantum materials**, including materials with unusual electronic states that are relevant for future electronics and quantum technologies. It clarified the behavior of difficult oxide materials such as rare-earth nickelates, and it helped explain materials in which electric and magnetic properties are linked. These are landmark contributions because they turned long-standing scientific puzzles into clearer design rules.

MARVEL also worked on problems with direct societal relevance. Its teams studied materials for **solar cells**, **water splitting**, **batteries and solid-state ion conductors**, **nanoporous materials** for catalysis and separation, **molecular crystals** relevant to chemistry and pharma, and **advanced alloys** for high-performance manufacturing. In later years, the portfolio expanded further toward aerospace alloys, spectroscopy, automated experiments and hybrid quantum-classical algorithms.

Just as important, MARVEL changed *how* such science is done. Over the course of the NCCR, machine learning moved from a promising add-on to a core research tool. It was used not only to speed up atomistic simulations, but also to predict more complex properties such as spectra, chemical environments, electronic structure and diffusion. By the end of the funding period, MARVEL had shown that workflows can connect simulations, data handling and experiments in one reproducible chain — and in some cases even help drive experiments on automated platforms.

A lasting Swiss infrastructure for digital materials research

MARVEL did not only produce papers. It also built a durable **Swiss research infrastructure**. What began as a network centered at EPFL and involving ETH Zurich, PSI, Empa, CSCS, and partner universities, evolved into a national platform for digital materials science. That matters because the real legacy of a NCCR is not only what it discovers during its funding period, but what it leaves behind for the next decade.

The clearest example is the open digital ecosystem built around **AiiDA/AiiDAlab**, **Materials Cloud**, **Quantum Mobile**, the **Materials Cloud *Learn*** and **Lhumos** platforms and later educational tools such as **OSSCAR**. In plain terms, these tools make complex simulations easier to run, easier to reproduce, easier to share and easier to teach. They help researchers keep track of how a result was produced, compare results from different simulation engines, publish reusable datasets, and turn expert workflows into tools that many more people can use.

This digital infrastructure became internationally visible in its own right. The Materials Cloud grew from a project platform into a recognized open repository and public service. It now hosts curated data, online tools, workflows and teaching material for a worldwide community, and it reached its 1'000th *Archive* record in 2024. Open access to data is unique worldwide, with complete and beyond-FAIR provenance tracking. Open access to publications also became routine inside the NCCR, which means that MARVEL's results are not locked behind closed systems but can be reused by researchers, teachers and innovators.

The structural legacy is also institutional. MARVEL helped anchor long-term capacity at PSI through the **Laboratory for Materials Simulations** and the wider **Scientific Computing, Theory and Data** effort. It also strengthened computational activities at Empa and supported new hires and cross-institutional appointments. By the final phase, the NCCR deliberately concentrated resources on the assets most likely to last beyond the funding period: digital infrastructure, long-term theory–experiment integration, and stable institutional homes.

From science to use: open science, industry and public value

MARVEL treated **open science** as part of the research process itself, not as an afterthought. Data behind publications were increasingly deposited in open repositories, software was released in open form whenever possible, and researchers were actively trained to meet open-access requirements. This created value both inside and outside the consortium: it improved quality and reproducibility, while also allowing other groups to build on MARVEL's work.

Knowledge and technology transfer followed the same logic. In MARVEL, transfer did not only mean patents. It also meant open-source software, reusable workflows, better interfaces between academic and industrial research, and the movement of trained people into companies and public laboratories. The NCCR built ties with a large industrial community across energy, electronics, metals, chemistry, catalysis and pharma. Over the years, it had contact with **dozens of companies** and signed several collaborations, with almost **CHF 7 millions** in funding. A particularly important achievement was the move from software development for experts to practical tools that can be adopted in industrial settings. AiiDA workflows, AiiDAlab applications and common workflows created a bridge from frontier research to everyday use. MARVEL also used **Industry Sector Days** to listen to companies, understand what they need, and position its work where it could have the greatest long-term value. These activities were deliberately pre-competitive: the goal was to strengthen capability and readiness for innovation, not only to solve one immediate industrial problem.

MARVEL's public **communication & outreach** was equally strong. It invested in a professional website, regular newsletters, feature stories and science highlights, press releases, social media and public events. By 2026, the website hosts more than **170 science highlights or feature stories** and more than **260 news items**, while the NCCR has issued **61 press releases** through EurekAlert since 2019. Public events such as Open Days, school visits, science festivals, the Ig Nobel Award Tour Show, and distinguished lectures helped explain a highly technical field in ways that non-specialists could enjoy and understand.

People, fairness and the next generation

A major strength of MARVEL was its investment in people. The NCCR created a rich training environment for PhD students, postdocs, Master students and even high-school students. Monthly junior seminars, junior retreats, summer schools, coding weeks and tutorials built a real community across institutions. The **Materials Cloud *Learn*** and **Lhumos** platforms turned many of these activities into lasting online resources, while lecture series such as the **CECAM-MARVEL Classics** made expert knowledge accessible to wider audiences. This **education and training** effort extended well beyond the core consortium. MARVEL supported a summer camp for high-school students, contributed to international schools, and helped sustain the **ASESMA** network for electronic-structure training in Africa. In other words, the NCCR trained researchers at different career stages and also invested in the broader pipeline of future talent.

MARVEL also treated **equal opportunities** as a strategic priority. The NCCR recognized early that women remain underrepresented in the disciplines on which MARVEL depends, and it responded with concrete measures. The best-known example is the **INSPIRE Potentials** program, launched in 2016 to fund six-month Master's research projects for women students in MARVEL laboratories. After 20 rounds, the program had supported **62 fellows** across **24 groups** and **8 institutions**; **19** of these fellows later continued at PhD level in MARVEL or former MARVEL groups, while at least **24** continued their careers in related fields elsewhere. This effort was part of a broader culture change. The number of women PhD researchers in the NCCR doubled during phase II, and targeted **Agility Plus** calls brought additional women principal investigators into the network. MARVEL also organized bias-awareness and leadership workshops, supported outreach activities for girls, took part in the **#NCCRWomen** campaign, and helped create visible role models through public portraits, interviews and events. These actions matter because a stronger research system is not only one that produces excellent science, but also one that becomes more open, fair and attractive to future talent.

Overall significance

Taken together, MARVEL's achievements across research, structure, knowledge and technology transfer, equal opportunities, education and training, communication & outreach, and open science tell one consistent story. The NCCR helped turn computational materials science in Switzerland into a field that is **faster**, **more reproducible**, **more open**, **better connected to experiments**, and **more visible internationally**. It leaves behind new scientific understanding, public digital infrastructure, lasting institutional homes, industrial links, trained researchers and a more inclusive culture.

Several examples make this legacy tangible. A researcher in Switzerland or abroad can now learn a method on Materials Cloud, run a reproducible workflow through AiiDA, inspect the data behind a paper, and reuse tools first built inside MARVEL. A company can engage with a community that already speaks both the language of frontier simulation and the language of practical adoption. A student can enter the field through a summer camp, a tutorial, a Master's fellowship or a junior seminar, and then continue into doctoral research. And a laboratory at PSI or Empa can build on structures that were strengthened during the NCCR instead of starting from scratch.

What remains after the funding period

Several parts of MARVEL are already larger than the original project and are likely to remain useful well beyond the funding period:

Public digital infrastructure that keeps data, workflows, online tools and educational material available to the international community.

Institutional hubs in Switzerland, especially at PSI, Empa and EPFL, that can continue advanced materials simulations and theory–experiment collaboration.

A trained talent pipeline of students, postdocs and young group leaders who learned to work across disciplines rather than inside isolated specialties.

Working relations with industry and public stakeholders that make future innovation faster and more credible.

A stronger public profile for the field, built through outreach, media work, school engagement and visible role models.

That combination is the real legacy of MARVEL. It is not only a successful research program from the past. It is a platform that should continue to shape how materials are discovered, shared and used in Switzerland and beyond.

2 Structural development and available resources

This chapter reviews the structural trajectory of NCCR MARVEL from its launch in 2014 to its late phase-III legacy strategy. MARVEL evolved from a matrix of vertical, horizontal and platform projects into a portfolio of design-and-discovery programs, and finally into a deliberately legacy-oriented structure centered on digital infrastructure and long-term Swiss embedding. Its achievement is a distributed national architecture linking EPFL, ETH Zurich, PSI, Empa, CSCS, and Swiss universities through shared governance, common workflows, open data platforms, coordinated training, and theory-experiment partnerships. The strongest post-NCCR assets are now visible in durable structures, such as the Materials Cloud, AiiDA/AiiDAlab, the Laboratory for Materials Simulations and the wider Scientific Computing, Theory and Data division at PSI, the consolidation of computational activities at Empa, and a new generation of junior researchers and professors recruited into Swiss institutions. We also note where ambitions had to be narrowed or delayed, especially under tighter phase-III funding, changing personnel, and the difficulty of converting exploratory initiatives into permanent structures, and argue that MARVEL's legacy is best classified as a national network with strong digital infrastructure and institutional hubs.

2.1 Structural starting point and development of the NCCR

A national computational network

The NCCR MARVEL began in May 2014 with EPFL as the home institution and an initial network spanning eleven Swiss academic and industrial institutions: EPFL, ETH Zurich, the Universities of Geneva, Fribourg, Basel and Zurich, Università della Svizzera italiana, CSCS, PSI, Empa and IBM Research Zurich. Scientifically, the center was organized around two vertical projects, novel materials physics (VP1) and novel materials applications (VP2), supported by three horizontal projects in advanced quantum simulations (HP3), advanced sampling methods (HP4) and materials informatics (HP5), and interfaced with two platform projects devoted to informatics and high-performance computing (PP6) and to experimental synthesis, characterization and testing (PP7). Governance was stratified through an Executive Committee, a Scientific Committee, and a Scientific Advisory Board. The initial scientific base was compact and strongly computational, but already national in reach and explicitly linked to experiments through PP7.

MARVEL was from the outset designed as a Swiss network in which the national laboratories (PSI and Empa) and CSCS were constitutive partners. The structure also mirrored a design and discovery pipeline. Fundamental physics and applications were linked to algorithms, data management, high-performance computing (HPC) and experimental validation. In that sense, the NCCR started from a stronger integration logic than a conventional multi-PI consortium. The preparatory period before the official launch, which included joint code development, a community workshop and a junior retreat, already shows that the center's leaders understood community formation and shared technical infrastructure as preconditions for scientific success.

Multidisciplinary and institutional expansion

From the beginning, MARVEL used competitive calls and targeted appointments to enlarge both its group base and its disciplinary palette. Experimental participation expanded markedly through PP7. A first round of additional group leaders was launched early in the program, bringing the total number of group leaders from 24 to 33, and a second wave of 6 experimental leaders followed. This had the effect to moved experiment from the status of external validator to that of embedded part-

Phase	Core structure	Measures to build the network	Structural effect
Phase I	2 vertical, 3 horizontal and 2 platform projects; Executive Committee, Scientific Committee, and Scientific Advisory Board	Full-time hiring policy for NCCR personnel, PP7 experimental calls, annual Review and Retreat, junior retreats, common regulations, early AiiDA and HPC agreements;	Established a nationally distributed but coherent computational materials network with explicit experiment and informatics interfaces.
Late phase I	Matrix structure retained but enlarged	UniBE joined; Executive Committee expanded; second wave of PP7 leaders; review-panel-driven collaborative grants and Agility Plus projects;	Broadened the network in personnel and disciplines and intensified cross-group collaboration, especially around junior-led and newly arrived investigators.
Phase II	6 D&D projects, 2 Incubators, Open Science Platform and HPC and Future Architectures Platform; Strategic Committee and Industrial Advisory Board added	Larger collaborative projects, industry sector days, data team, RDM strategy, INSPIRE Potentials fellowships, tutorials and coding weeks;	Shifted MARVEL from a field-based matrix to mission-oriented collaborative programs and elevated digital infrastructure to a core structural function.
Phase III	Pillars 1 to 4, Advanced Simulation Methods, and Quantum Simulations	Focus on post-2026 embedding, PSI and Empa anchoring, partnership with CSCS, new hires, one-to-one PI meetings, and stronger EU/platform federation;	Concentrated the NCCR around legacy-bearing assets: digital infrastructure, long-term Swiss integration, and a renewed cohort of researchers and institutional homes.

Table 2.1: Phase-wise evolution of NCCR MARVEL as a scientific and structural network.

ner and gave MARVEL deeper access to synchrotron science, spectroscopy, catalysis, synthesis and characterization, in particular at PSI and Empa.

Institutionally, the network broadened again in late phase I when the University of Bern joined in January 2017, taking the participating institutions to twelve. At the same time, MARVEL used Agility Plus funding to bring in researchers such as Ulrich Aschauer (UniBE), William Curtin (EPFL), and Martin Jaggi (EPFL). This renewal followed the recommendations of the review panel that new funding should privilege collaborative projects led by junior or recently arrived personnel and should prepare the scientific portfolio for phase II. The redistributed CHF 1 million acted as an internal renewal mechanism that made the network more open to new expertise and more explicitly collaborative (Table 2.1).

The disciplinary profile broadened in parallel. Phase I was anchored in computational condensed-matter physics, theoretical chemistry, atomistic simulations, advanced sampling, materials informatics, high-performance computing and experiment. By phase II, MARVEL had substantially strengthened machine learning, porous materials and MOFs, structural metals and alloy design, low-dimensional materials and nanoelectronics, solid-state ionics, data stewardship and open-science engineering. By phase III, further layers had become explicit in the structure itself, with a machine-learning platform for molecules and materials, a digital infrastructure of open simulations and data, advanced simulation methods for correlated materials and devices, and quantum algorithms for materials discovery. In structural terms, the center evolved from a federation of disciplines into an organization in which software engineering, FAIR data, automation, computational spectroscopy, and education became constitutive elements of the research program (chapter 3).

Three phases of structural redesign

MARVEL's most distinctive structural feature is that it repeatedly redesigned itself in response to what the science demanded. In phase I, the vertical-horizontal-platform matrix was a sensible way to establish common language, shared methods and common infrastructure across distinct domains. By the end of phase I, however, it had become clear that the center's strongest results were emerging from larger thematic constellations. This triggered a major restructuring in phase II, with six Design & Discovery (D&D) projects and two Incubators, supported by an Open Science Platform and an HPC and Future Architectures Platform. Governance evolved in parallel, with an enlarged Executive Committee, a Strategic Committee formalizing funding reallocations, and an Industrial Advisory Board complementing the Scientific Advisory Board

(Table 2.1).

This redesign aligned the formal organization with the actual collaboration patterns that MARVEL had generated. It also elevated the Open Science Platform, the home of the Materials Cloud, AiiDA and related tools, to the status of a central structural effort. Phase III brought a second redesign. With the funding reduction, the NCCR chose concentration over breadth. Several phase-II PIs did not continue, and the consortium was reorganized into four pillars, an advanced simulation methods project and a quantum simulations bonus project. Pillar 3 made digital infrastructure itself a legacy target, while Pillar 4 explicitly addressed long-term integration in the Swiss scientific landscape. With this, MARVEL's final phase turned structural legacy from an outcome into an organizing principle (Table 2.1).

Building a collaborative network

MARVEL invested continuously in mechanisms that converted a set of groups into a functioning community. One recurring principle was the policy of hiring researchers fully into NCCR projects whenever possible. This created a clear MARVEL identity and reduced the fragmentation that often occurs when staff are only partially associated with a large consortium. Another recurring measure was the use of repeated face-to-face and later hybrid or online interactions: annual Reviews and Retreats, project meetings, junior retreats, junior seminars, distinguished lectures, CECAM-MARVEL series, AiiDA tutorials, coding weeks, industry sector days and mixed experimental-computational events. These formats built real collaborations at all levels, from PIs to students, and especially between EPFL, ETH Zurich, PSI, Empa and CSCS.

A second family of measures concerned procedural maturation. MARVEL progressively formalized internal regulations, built a management team with responsibility for equal opportunities, knowledge and technology transfer, education and training, and communication, and later created a data team and a research-data-management (RDM) strategy. In phase III it also updated crisis communication procedures and internal regulations (Table 2.1). These were not peripheral administrative refinements. In a consortium of this size, shared norms for authorship acknowledgment, data deposition, platform usage, outreach and diversity directly affected the center's ability to work coherently across institutions.

MARVEL also used selective renewal mechanisms to keep the network dynamic. Agility Plus projects, PP7 experimental calls, budget reallocations and the targeted admission of new PIs all served as controlled ways of bringing new ideas and people into the NCCR without destabilizing the whole structure. This is one reason why structural development contributed so directly to scientific achievements. Collaboration was not left to chance or goodwill alone. It was scaffolded by governance, personnel policy, recurrent events, shared digital infrastructure and flexible internal funding instruments.

2.2 Structural impact and perspectives beyond the NCCR

Core structural impacts and educational capacity

The NCCR's clearest structural impact lies in the creation of durable research platforms. The open science platform and its predecessor grew into a mature ecosystem around Materials Cloud, AiiDA/AiiDAlab, Quantum Mobile, common workflows, discoverable datasets and educational resources. Materials Cloud moved from a dissemination idea to a public platform with *Learn*, *Work*, *Discover*, *Explore* and *Archive* sections, DOI minting, long-term storage, provenance-aware browsing, web apps and scalable backends. AiiDA evolved in parallel from workflow engine to widely used open-source provenance infrastructure, with plugins, common workflows and interfaces to many electronic-structure codes (Table 2.2). By phases II and III, these elements had become community infrastructure with international users, FAIR-data visibility, GO FAIR participation, and growing links to core European projects such as MaX and BIG-MAP (and, most recently, Materials Commons), plus a host of other EU projects aligned on the digital infrastructure (MarketPlace, NFFA, INTERSECT, OpenModel, Dome 4.0).

MARVEL also had structural impact through appointments and institutional design. The phase-II and phase-III periods saw targeted hires or integrations that clearly outlived the logic of a normal project grant: William Curtin strengthened the center's capability in structural metals, Agility Plus brought in new female PIs and broadened the disciplinary base, and phase III introduced or consolidated a new cohort of researchers including Anirudh Raju Natarajan, Giuseppe Carleo, Sara Bonella, Michael Schüler, Zoë Holmes and Michael Herbst. Two cases are structurally especially important. First, EPFL created a joint interfaculty chair in Math and Materials, which made possible the recruitment of Michael Herbst. Second, UniFR and PSI jointly appointed Michael Schüler in light-matter interactions, explicitly linked to the new Laboratory for Materials Simulations at PSI (Table 2.5).

On the education side, the legacy is broad. The NCCR developed a layered training ecosystem embedded in the teaching and mentoring environments of the participating institutions, mostly captured in the Materials Cloud *Learn* and Lhumos platforms. This included AiiDA and high-throughput tutorials, coding weeks, junior seminars, junior retreats, distinguished lectures, summer camps for high-school students, conference fellowships and the INSPIRE Potentials master's fellowships for female students. Later, MARVEL also contributed to open educational infrastructure through OSSCAR notebooks and AiiDAlab-based tools (Table 2.2). Structurally, this approach was sensible for a distributed Swiss network, influencing curricula and skills formation across institutions without needing to found a separate degree program. This relevance became apparent at the outset of Covid 19, when the "Fireside chats for lockdown times" reached the limit of 500 Zoom participants in the five minutes before the start.

Implementation constraints and scope limitations

The clearest limitation in the structure was the need to concentrate resources. In phase II, reallocation to equal-opportunities measures and the front-loaded budget profile led to cuts in several projects and a particularly sharp reduction of the Incubator projects; Incubator 1 stopped at the end of year 7 and Incubator 2 continued only with reduced support. By phase III, the overall NCCR budget had decreased strongly relative to the previous phases, and many successful phase-II PIs no longer continued (Tables 2.6 and 2.8). MARVEL responded by keeping the strongest and most legacy-bearing activities, but the cost of that decision was a narrower consortium and the abandonment or reduction of some exploratory breadth.

Another limitation is that MARVEL's educational innovations, although substantial, remained modular rather than fully institutionalized. The NCCR created fellowships, online notebooks, schools and training series, but not a national graduate program or jointly governed curriculum. This was probably a rational choice for a multi-institutional network, yet it means that some educational gains will survive only if host institutions continue to resource them. The same is true for digital infrastructure. Materials Cloud and AiiDA/AiiDAlab have strong technical momentum, but their long-term health depends on research software engineers, platform developers, moderators and data stewards, professional profiles that are still not always securely funded in ordinary academic structures.

Post-funding sustainability

Regarding MARVEL's legacy logic, we can cite two examples.

The Materials Cloud is far more than a project website. It became a layered infrastructure with a public identity, international moderation and repository practices, technical backends, a user base and integration into wider European ecosystems. By 2018, all five sections were operational, by 2020, the platform had around 15'000 unique monthly visitors, more than 250 total *Archive* records, a migration to the scalable Invenio 3 backend and growing use beyond MARVEL. Later, CSCS delivered platform-as-a-service, federation of the *Archive* with CINECA and Jülich through MaX, strong ties to BIG-MAP and Battery2030+, and integration with experimental data environments and AiiDAlab. The strongest argument for continuity is therefore that Materials Cloud is embedded in three layers at once: in the software and data teams built within MARVEL, in a service partnership with CSCS, and in European platform ecosystems that extend well beyond the NCCR. The main risk is not scientific relevance but governance and staffing. Platform moderation, software maintenance and long-term data stewardship require sustained professional support; very positively CINECA has now dedicated two OS FTE positions to this.

The Laboratory for Materials Simulations at PSI is even more clearly positioned for survival. Pillar 4 in phase III was explicitly designed to phase in MARVEL's activities beyond 2026 through core partnerships with PSI and Empa. PSI created in July 2021 a new division dedicated to Scientific Computing, Theory and Data under Christian Rüegg. Within that

Type of structural aspect	**Details**
NCCR structures	• Paul Scherrer Institute (PSI): creation of a Center of Scientific Computing, Theory and Data), including a Laboratory for Materials Simulations (headed by Nicola Marzari), with ○ a group on Light-Matter interactions (Michael Schüler, joint with UniFR) ○ a group on Materials Software and Data (Giovanni Pizzi) ○ a group on Multiscale Materials Simulations (Matthias Krack) ○ two tenure-track scientists (Nicola Colonna and Iurii Timrov) • Empa: AiiDAlab has become a core and supported capability for different laboratories • CSCS: materials has become one of the two core communities/domains part of CSCS long-term structure and strategy; this includes the Materials Cloud Platform-as-a-Service (PaaS) and SIRIUS for pre-exascale and exascale deployment • Integration in many ongoing EU projects — notably Materials Commons and MaX • Creation of a domain-specific materials node (MatOSC) in the European Open Science Cloud (EOSC)
NCCR-Network	• See list on next two pages (Tables 2.3 and 2.4)
Collaborations NCCR-network	• Bonella + Pizzi (continuing) • Carleo + Holmes (continuing) • Carleo + Tavernelli • Ceriotti + Corminboeuf (continuing) • Ceriotti + Emsley (continuing) • Ceriotti + Marzari (continuing) • Ceriotti + Pizzi (continuing) • Laino + Marzari (continuing) • Luisier + Marzari (continuing) • Luisier + Passerone (continuing) • Marzari + Passerone (continuing) • Marzari + Pizzi (continuing) • Marzari + Pignedoli + Pizzi (continuing) • Passerone + Werner (continuing) • Pignedoli + Pizzi (continuing) • Schüler + Werner (continuing) • Georges + Werner • Herbst + Pizzi (new) • Corminboeuf + Pignedoli (new)
Educational programmes	• MARVEL junior retreat – continue if self-funding is agreed/found • MARVEL junior seminars – continuing with a team of junior researchers and funding from the MARVEL groups (Ceriotti, Corminboeuf, Bonella) • INSPIRE Potentials — MARVEL Master's fellowships — these have now become an established and widespread concept in many recent NCCRs; the spirit will also continue at EPFL with the MX Master fellowship program • INSPIRE visiting PhD fellowships – concluded • CECAM-MARVEL Classics in molecular and materials modelling and CECAM-MARVEL Mary Ann Mansigh Conversation series: continuation as CECAM series • MARVEL Distinguished Lectures – concluded (but these and all the MARVEL and CECAM-MARVEL events are permanently recorded/available on Materials Cloud *Learn* and Lhumos) • Summer camp for high school students – continue with secured funding from EPFL Education Outreach Department and EPFL Section of Materials (SMX) • Actions towards girls and young women – EPFL Science Outreach Department is continuing such activities generally and on MARVEL-related topics (materials science, chemistry, coding, etc.), at least for the upcoming years
Infrastructures / platforms	• Materials Cloud — data storage and services for the Materials Cloud are in place to support the platform at least till 2036 (i.e., guaranteeing at least 10 years after submission), mostly deployed at CSCS, but with CINECA Bologna now taking over the *Archive* services with additional personal • Hardware for Materials Cloud (for Materials Cloud core deployment at EPFL & PSI): neither willing/able. New EU projects (e.g., Materials Commons) and future initiatives providing continuing support • High-performance computing at CSCS • AiiDA / AiiDAlab • Lhumos • CoViz2 Distance Learning Room – EPFL will keep maintaining it

Table 2.2: *Structural achievements (data from: April 2026). List of achievements.*

Computational PIs			
PI name	**In MARVEL**	**Projects**	**Left to**
Wanda Andreoni (EPFL)	Year 1 to year 3	Phase I, VP2	Retired
Ulrich Aschauer (UniBE)	Year 3 to year 8	Phase I, VP1 / Phase II, DD5	Department of Chemistry and Physics of Materials, Paris-Lodron University Salzburg (AT)
Sara Bonella (EPFL)	From year 9	Phase III, P3	
Giuseppe Carleo (EPFL)	From year 9	Phase III, QS	
Michele Ceriotti (EPFL)	Full period	Phase I, HP5 / Phase II, DD1 & DD2 / Phase III, P2	
Volkan Cevher (EPFL)	Year 2 to year 4	Phase I, HP5	
Clémence Corminboeuf (EPFL)	Full period	Phase I, VP2 / Phase II, DD1 / Phase III, P2	
Alessandro Curioni (IBM)	Year 1 to year 4	Phase I, HP5	
William Curtin (EPFL)	Year 4 to year 10	Phase I, VP2 / Phase II, DD2 / Phase III, P1	Retired
Claude Ederer (ETHZ)	Year 5 to year 8	Phase II, DD5	
Antoine Georges (UniGE)	Year 1 to year 4	Phase I, VP1	Flatiron Institute, Director, CCQ, New York (USA)
Stefan Goedecker (UniBas)	Year 1 to year 8	Phase I, HP4 / Phase II, DD1	
Michael Herbst (EPFL)	From year 10	Phase III, P3	
Zoë Holmes (EPFL)	From year 10	Phase III, QS	
Jürg Hutter (UZH)	Full period	Phase I, HP3 / Phase II, DD4 / Phase III, QS	
Martin Jaggi (EPFL)	Year 4	Phase I, HP5	
Christoph Koch (EPFL)	Year 1 to year 4	Phase I, HP5	
Teodoro Laino (IBM)	Year 5 to year 7	Phase II, Inc1	
Mathieu Luisier (ETHZ)	From year 4	Phase II, DD3 / Phase III, ASM	
Nicola Marzari (EPFL + PSI)	Full period	Phase I, VP2 / PP6 / Phase II, DD3 & Inc1 & OSP / Phase III, P4	Cavendish Professor of Physics, University of Cambridge (UK)
Titus Neupert (UZH)	Year 6 to year 8	Phase II, DD6	
Michele Parrinello (USI)	Year 1 to year 8	Phase I, HP4 / Phase II, DD1	Italian Institute of Technology (IT)
Alfredo Pasquarello (EPFL)	Year 1 to year 8	Phase I, VP2 / Phase II, DD3 & DD4	
Daniele Passerone (Empa)	Full period	Phase I, VP2 / Phase II, DD3 / Phase III, ASM	
Carlo Pignedoli (Empa)	From year 9	Phase III, P4	
Giovani Pizzi (PSI)	From year 5	Phase II, OSP / Phase III, P3	
Anirudh Raju Natarajan (EPFL)	From year 9	Phase III, P1	
Volker Roth (UniBas)	Year 5 to year 7	Phase II, Inc2	
Ursula Röthlisberger (EPFL)	Year 1 to year 4	Phase I, VP2	
Michael Schüler (UniFR + PSI)	From year 9	Phase III, ASM	
Thomas Schulthess (CSCS)	Year 1 to year 8	Phase I, PP6 / Phase II, HPC	
Berend Smit (EPFL)	Year 1 to year 10	Phase I, HP4 / Phase II, DD4 / Phase III, P1	
Alexey Soluyanov (UZH)	Year 5 to year 6	Phase II, DD6	Passed away 2019
Nicola Spaldin (ETHZ)	Year 1 to year 8	Phase I, VP1 / Phase II, DD5	
Ivano Tavernelli (IBM)	From year 5	Phase II, DD4 / Phase III, QS	
Matthias Troyer (ETHZ)	Year 1 to year 4	Phase I, VP1	Technical Fellow and Corporate Vice President of Quantum, Microsoft, Redmond, WA (USA)
Vladyslav Turlo (Empa)	From year 9	Phase III, P1	
Joost VandeVondele (CSCS)	Full period	Phase I, HP3 / Phase II, HPC / Phase III, P3	
Anatole von Lilienfeld (UniBas)	Year 1 to year 8	Phase I, HP5 / Phase II, Inc2	Professor, Department of Materials Science & Engineering, University of Toronto (CA)
Philipp Werner (UniFR)	Full period	Phase I, HP3 / Phase II, DD5 / Phase III, ASM	
Oleg Yazyev (EPFL)	Year 1 to year 8	Phase I, VP1 / Phase II, DD6	
Lenka Zdeborová (EPFL)	From year 9	Phase III, P2	

Table 2.3: *Structural achievements (data from: April 2026). NCCR-Network, computational PIs.*

division, the Laboratory for Materials Simulations was developed in close partnership with MARVEL and led by Nicola Marzari through a temporary 20% PSI appointment. The laboratory comprises a Materials Software and Data group, a Multiscale Materials Modelling group, and a Light-Matter Interactions line strengthened by the joint UniFR-PSI appointment of Michael Schüler. Moreover the MARVEL efforts there are cash matched by PSI and Empa. This is precisely the kind of embedding expected from a successful NCCR, a durable

Experimental PIs			
PI name	**In MARVEL**	**Projects**	**Left to**
Ana Akrap (UniFR)	Year 7 to year 9	Phase II, AG+ - DD6	Professor, Physics Department of University of Zagreb (HR)
Raffaella Buonsanti (EPFL)	Year 3 to year 4	Phase I, PP7	
Claudia Cancellieri (Empa)	Year 2 to year 3	Phase I, PP7	
Lyndon Emsley (EPFL)	From year 7	Phase II, DD1 / Phase III, P2	
Emiliana Fabbri (PSI)	Year 7 to year 9	Phase II, AG+ - DD4	
Roman Fasel (Empa)	Year 5 to year 8	Phase II, DD3	
Marta Gibert (UZH)	Year 7 to year 9	Phase II, AG+ - DD5	Professor, Institute of Solid State Physics, TU Wien (AT)
Pierangelo Gröning (Empa)	Year 1 to year 4	Phase I, PP7	
Michel Kenzelmann (PSI)	Year 1 to year 8	Phase I, PP7 / Phase II, OSP	
Christian Leinenbach (Empa)	From year 9	Phase III, P1	
Thomas Lippert (PSI)	Year 2 to year 3	Phase I, PP7	
Piero Macchi (UniBE)	Year 5 to year 6	Phase II, DD4	Professor, Dipartimento di Chimica, Materiali e Ingegneria Chimica, Politecnico di Milano (IT)
Marisa Medarde (PSI)	Years 2, 3, 5 to 7	Phase I, PP7 / Phase II, DD5	
Frithjof Nolting (PSI)	Year 1 to year 4	Phase I, PP7	
Daniele Pergolesi (PSI)	Year 3 to year 7	Phase I, PP7 / Phase II, Inc1	
Wendy Queen (EPFL)	Year 3 to year 4	Phase I, PP7	
Marco Ranocchiari (PSI)	Year 3 to year 4	Phase I, PP7 / Phase II, DD4	
Sereina Riniker (ETHZ)	Year 7 to year 9	Phase II, AG+ - DD1	
Marta Rossell (Empa)	Year 3 to year 4	Phase I, PP7	
Christian Rüegg (PSI)	Year 3 to year 4, from year 9	Phase I, PP7 / Phase III, P4	
Thomas Schmidt (PSI)	Year 2 to year 3	Phase I, PP7	
Thorsten Schmitt (PSI)	Year 2 to year 3	Phase I, PP7	
Ming Shi (PSI)	Year 3 to year 4	Phase I, PP7 / Phase II, DD6	Professor, Center for Correlated Matter and School of Physics, Zhejiang University, Hangzhou (CN)
Grigory Smolentsev (PSI)	Year 2 to year 3	Phase I, PP7	
Urs Staub (PSI)	Year 2 to year 3	Phase I, PP7 / Phase II, DD5	
Kyriakos Stylianou (EPFL)	Year 5 to year 6	Phase II, DD4	Professor, Department of Chemistry, Oregon State University (USA)
Dirk van der Marel (UniGE)	Year 2 to year 3	Phase I, PP7	
Claire Villevieille (PSI)	Year 5 to year 6	Phase II, Inc1	Research director @ CNRS, Grenoble INP - UGA, Graduate schools of Engineering and Management (FR)

Table 2.4: *Structural achievements (data from: April 2026). NCCR-Network, experimental PIs.*

laboratory with personnel, groups, an institutional parent division and a clear mission in Swiss computational materials science.

Collaboration beyond the funding period is therefore likely to be maintained through a distributed but anchored model. EPFL remains the main academic home for several PIs, educational initiatives and scientific directions. PSI provides the most explicit long-term laboratory and divisional framework for simulation, software and spectroscopy. Empa offers complementary embedding on the experimental and computational side. CSCS remains the backbone for HPC and platform delivery. The network may become leaner after the NCCR, but it should also become more institutionally normalized (Tables 2.2 and 2.5).

The structural legacy of MARVEL

MARVEL's legacy can be understood as a *distributed national network legacy with strong institutional hubs and a durable digital infrastructure layer*. Indeed, MARVEL reshaped the internal profile of its home institution EPFL by consolidating one of Europe's most visible clusters in computational materials design and discovery. It also contributed directly to the creation or strengthening of durable institutional homes beyond EPFL, above all the Laboratory for Materials Simulations and the wider PSI division, and the consolidation of computational activities at Empa. It finally created national and international digital infrastructures, Materials Cloud, AiiDA/AiiDAlab, common workflows and open educational tools, that are portable across institutions and communities.

The remaining challenges follow from the

Type of structural position	Output
Number of created professorships per type	**1 new full professor** • Berend Smit (EPFL, 2014) **6 new assistant professors (**all tenure track) • Oleg Yazyev (EPFL, 2011) • Michele Ceriotti (EPFL, 2013) • Martin Jaggi (EPFL, 2015) • Anirudh Raju Natarajan (EPFL, 2022) • Michael Herbst (EPFL, 2022) • Michael Schüler (UniFR + PSI, 2022) **2 successions / replaced positions** (within NCCR field) • Planned junior hire in EPFL IMX to substitute Nicola Marzari • Planned senior hire between EPFL IMX and PSI to substitute Nicola Marzari **Hired in the topic of MARVEL and involved in the project:** • Lenka Zdeborová (as associate professor) • Giuseppe Carleo (as PATT) • Zoë Holmes (as PATT)
Sustainability of professorships	**Created professorships during the time of MARVEL** • Tenured (associate professor): Yazyev, Jaggi, Carleo • Tenured (associate professor) and then appointed to full professor: Ceriotti **Development of professorships already existing at the start of MARVEL** • Tenured (associate professor) and then appointed to full professor: Volkan Cevher • Associate professor appointed to full professor: Clémence Corminboeuf
Junior Group Leaders	**4 tenure-track group leaders / senior scientists (supported within NCCR)** • Giovanni Pizzi (EPFL, then PSI) • Iurii Timrov (EPFL, then PSI) • Nicola Colonna (PSI) • Aliaksandr Yakutovich (Empa) **3 software engineers** • Simon Pintarelli (CSCS) • Guillaume Fraux (EPFL, SCITAS) • Roberto Bendinelli (EPFL, CECAM)
Careers Junior Group Leaders	• Daniele Passerone (Empa) was appointed as adjunct professor at ETH Zurich

Table 2.5: Structural positions and recruitments (data from: April 2026).

same distributed character. A network legacy can dissipate if the incentives of the host institutions drift apart, if platform maintenance lacks stable funding, or if leadership succession is not planned. In MARVEL's case, the most important challenges are the long-term resourcing of research software engineering and data stewardship, maintaining tight theory-experiment coupling once NCCR-specific coordination budgets disappear, and ensuring that the platforms remain community services rather than underfunded side projects of a few laboratories. These are real challenges, but they are the challenges of a successful structural legacy.

2.3 Financial resources and personnel

Over the twelve years duration of the NCCR MARVEL, the total funding from SNSF was 48 MCHF, complemented by self-funding and 3rd party funding of 76 MCHF (Table 2.6). The allocation of the SNSF funding by PI throughout the phases is reported in Table 2.8. PIs SNSF funding was used almost entirely for salaries (PhD students and postdocs, mainly). 1.5 MCHF in phase I and 1.7 MCHF in phase II (HPC Provisioning in Table 2.8) were invested

Funding source		Phase I	Phase II	Phase III	All phases
SNSF Funding	Cash	17’458’355	16’905’739	13’676’010	48’040’104
Self-funding Home Institution	Cash	2’478’527	1’982’652	1’590’831	6’052’010
	In-kind	3’195’634	2’250’302	2’264’081	7’710’017
Self funding from project participants	Cash	35’620	5’077	0	40’697
	In-kind	19’724’455	20’487’652	14’755’654	54’967’761
Self-funding other	Cash	0	0	0	0
	In-kind	2’132’668	1’270’881	2’096’495	5’500’044
3rd party funding	Cash	331’602	174’563	0	506’165
	In-kind	256’123	621’054	657’895	1’535’072
Total	Cash	20’304’104	19’068’031	15’266’841	54’638’976
	In-kind	25’308’880	24’629’889	19’774’125	69’712’894
	Total	45’612’984	43’697’920	35’040’966	124’351’870

Table 2.6: *Overall funding — expenses (data from: April 2026).*

Funding source	Phase I	Phase II	Phase III	All phases
Office (general management) and Open science	1’736’911	1’610’185	2’168’257	5’515’353
Education and training	337’236	272’850	169’077	779’163
Knowledge and technology transfer	383’710	241’935	14’391	640’036
Equal opportunities	142’312	317’734	316’418	776’464
Communication & outreach	571’182	612’805	750’178	1’934’165
Total	3’171’351	3’055’509	3’418’321	9’645’181

Table 2.7: *Management activities — expenses per phase all funding sources (data from: April 2026).*

in computing infrastructure at CSCS. The rest of the SNSF funding was used in the management areas. “Self-funding from project participants” matched the “SNSF funding” in each phase. “Self-funding other” includes the support of PSI and Empa, matching in cash the SNSF funding. This was part of the commitment PSI for the three phases of the project and of Empa for phases II and III. Part of the “Self-funding other” in phase III is also from CECAM. In addition to the “3rd party funding” to MARVEL reported in the table, the project continuously benefited from collaborations and cooperations with industrial partners as well as many and major European projects and grants, all of which are reported in the “Self-funding from project participants”, in-kind category. Non-SNSF funding contributed to more than 60% of the overall NCCR budget over the 12 years.

The management team stayed small throughout the project, with a scientific manager (60%), a program manager (60 to 100%), a finance officer (80%), an administrative assistant (50 to 70%), a KTT officer (20%, until November 2020), and a communication officer (20%). Their salaries were covered mostly by “Self-funding Home Institution” (cash and in kind), and partly in phase III with SNSF funding. Table 2.7 reports the expenses of the management activities, including the salaries, all funding sources combined. Some of the expenses reported as “Office” could be reported more precisely to one of the management areas (education and training, knowledge and technology transfer (KTT), equal opportunities, communication & outreach, open science). While the phase III KTT expenses look underestimated, in realty when the industrial liaison officer left in November 2020, the work performed for KTT in the management team was reported in “Office”. The work was continued, mainly done by the program manager (in particular but not only, through the organization of the two Psi-k conferences) and the actual expenses for KTT were at a similar level as in the previous phases.

Project Leader	Institution	Phase I Allocation	Phase II Allocation	Phase III Allocation	Total Allocation
AKRAP	UniFR	-	120’000.00	-	**120’000.00**
ANDREONI	EPFL	187’046.95	-	-	**187’046.95**
ASCHAUER	UNIBE	120’144.30	386’200.00	-	**506’344.30**
BONELLA	EPFL	-	-	500’000.00	**500’000.00**
BUONSANTI	EPFL	106’000.00	-	-	**106’000.00**
CARLEO	EPFL	-	-	600’000.00	**600’000.00**
CANCELLIERI	Empa	126’000.00	-	-	**126’000.00**
CEHVER	EPFL	248’505.82	-	-	**248’505.82**
CERIOTTI	EPFL	459’899.15	692’318.00	1’300’000.00	**2’452’217.15**
CORMINBOEUF	EPFL	406’496.20	692’318.00	1’000’000.00	**2’098’814.20**
CURIONI	IBM	806’700.09	-	-	**806’700.09**
CURTIN	EPFL	104’500.00	636’457.00	400’000.00	**1’140’957.00**
EDERER	ETHZ	-	388’202.00	-	**388’202.00**
EMSLEY	EPFL	-	78’080.00	-	**78’080.00**
FABBRI	PSI	-	60’000.00	-	**60’000.00**
FASEL	Empa	-	173’080.00	-	**173’080.00**
GEORGES	UNIGE	393’527.38	-	-	**393’527.38**
GIBERT	UZH	-	120’000.00	-	**120’000.00**
GOEDECKER	UNIBAS	654’867.22	441’160.00	-	**1’096’027.22**
HERBST	EPFL	-	-	200’000.00	**200’000.00**
HOLMES	EPFL	-	-	200’000.00	**200’000.00**
HPC Provisioning	CSCS	1’500’000.00	1’700’000.00	-	**3’200’000.00**
HUTTER	UZH	603’299.97	519’238.00	300’000.00	**1’422’537.97**
Inspire Potentials Master Fellowships	EPFL	201’300.00	457’000.00	350’734.33	**1’009’034.33**
JAGGI	EPFL	68’300.00	-	-	**68’300.00**
KOCH	EPFL	313’417.31	-	-	**313’417.31**
LAINO	IBM	-	268’080.00	-	**268’080.00**
LEINENBACH	Empa	-	-	120’000.00	**120’000.00**
LIPPERT	PSI	106’000.00	-	-	**106’000.00**
LUISIER	ETHZ	40’000.00	380’000.00	200’000.00	**620’000.00**
MACCHI	UNIBE	-	63’334.00	-	**63’334.00**
MARZARI	EPFL	795’392.71	780’517.00	-	**1’575’909.71**
MARZARI AND RUEGG (PSI)	EPFL	-	235’000.00	1’600’000.00	**1’835’000.00**
PP6.2 Materials informatics (software)	EPFL	1’468’203.99	-	-	**1’468’203.99**
Materials Cloud	EPFL	155’654.19	122’728.00	4’907.50	**283’289.69**
MEDARDE	PSI	131’000.00	102’000.00	-	**233’000.00**
PARRINELLO	ETHZ	672’402.75	363’080.00	-	**1’035’482.75**
PASQUARELLO	EPFL	760’000.00	665’278.00	-	**1’425’278.00**
PASSERONE	Empa	459’635.64	346’160.00	200’000.00	**1’005’795.64**
PERGOLESI	PSI	106’000.00	204’000.00	-	**310’000.00**
PIGNEDOLI	Empa	-	-	400’000.00	**400’000.00**
PIZZI	EPFL	-	2’630’000.00	1’300’000.00	**3’930’000.00**
QUEEN	EPFL	53’000.00	-	-	**53’000.00**
RAJU NATARAJAN	RPFL	-	-	400’000.00	**400’000.00**
RANOCCHIARI	PSI	53’000.00	115’388.00	-	**168’388.00**
RINIKER	ETHZ	-	120’000.00	-	**120’000.00**
ROETHLISBERGER	EPFL	657’771.68	-	-	**657’771.68**
ROSSELL	Empa	106’000.00	-	-	**106’000.00**
RUEGG	PSI	106’000.00	-	-	**106’000.00**
RUEGG	PSI	25’500.00	-	-	**25’500.00**
SCHMIDT	PSI	126’000.00	-	-	**126’000.00**
SCHMITT	PSI	118’000.00	-	-	**118’000.00**
SCHÜLER	UniFR	-	-	200’000.00	**200’000.00**
SCHULTHESS	CSCS	576’895.15	-	-	**576’895.15**
SHI	PSI	106’000.00	204’000.00	-	**310’000.00**
SMIT	EPFL	508’721.26	744’372.00	300’000.00	**1’553’093.26**
SMOLENTSEV	PSI	106’000.00	-	-	**106’000.00**
SOLUYANOV/NEUPERT	UNIZH	-	397’682.00	-	**397’682.00**
SPALDIN	ETHZ	649’504.20	190’000.00	-	**839’504.20**
STAUB	PSI	118’000.00	102’000.00	-	**220’000.00**
STYLIANOU	EPFL	-	63’334.00	-	**63’334.00**
TAVERNELLI	IBM	-	90’534.54	300’000.00	**390’534.54**
TROYER	ETHZ	794’482.00	-	-	**794’482.00**
TURLO	Empa	-	-	200’000.00	**200’000.00**
VAN DER MAREL	UNIGE	96’000.00	-	-	**96’000.00**
VANDEVONDELE	CSCS	196’158.85	655’615.46	700’000.00	**1’551’774.31**
VILLEVIEILLE	PSI	-	102’000.00	-	**102’000.00**
VON LILIENFELD	UNIBAS	492’197.38	709’238.00	-	**1’201’435.38**
WERNER	UNIFR	649’172.16	420’234.00	300’000.00	**1’369’406.16**
YAZYEV	EPFL	507’636.64	653’278.00	-	**1’160’914.64**
ZDEBOROVA	EPFL	-	-	200’000.00	**200’000.00**
Grand Total		**17’040’332.99**	**17’191’906.00**	**11’275’641.83**	**45’507’880.82**

Table 2.8: *Allocation by PI.*

2.4 Management and leadership

Interdisciplinary coordination

MARVEL's management model evolved in sophistication while keeping a clear principle: scientific leadership had to remain close to the research, but coordination had to be strong enough to make cross-institutional collaboration routine. In phase I, this was done through a small Executive Committee, supported by the Scientific Committee and the Scientific Advisory Board. In phase II, the Executive Committee was enlarged, a Strategic Committee took over explicit decisions on reallocations of funding, industrial advice was formalized through the Industrial Advisory Board, and management areas such as knowledge and technology transfer, education and training, equal opportunities and communication were assigned to named faculty and staff. By phase III, the Executive Committee combined scientific, infrastructural and strategic leadership, and one-to-one meetings with PIs complemented standard committee processes (Table 2.1).

This approach matched the real coordination problem. MARVEL was not only multidisciplinary, it linked groups that worked on very different timescales and with very different cultures, such as *ab initio* theorists, machine-learning developers, high-performance-computing specialists, software engineers, data-platform builders and experimental groups at PSI and Empa. Synergy had to be produced through repeated interaction, shared tools, visible incentives to collaborate and clear project-level responsibility. Annual reviews and retreats, junior retreats, tutorials, coding weeks, sector days and mixed experimental-computational meetings served this purpose. Collaborations emerged at all levels, between PIs, between postdocs and students, and between institutions such as PSI, Empa, EPFL, ETH Zurich and CSCS, and many of these collaborations would not have happened without MARVEL's coordination formats.

Major challenges

Several challenges recurred throughout the funding period. The first was how to bridge disciplinary distance. MARVEL dealt with this by progressively replacing a rigid work-package logic with larger collaborative programs and, later, pillars, each with a project leader responsible for integrating computational and experimental contributions. A second challenge was personnel volatility. Key scientists took leaves, moved institutions, retired, or in one tragic case passed away. The center responded by appointing co-leaders, reallocating budgets, maintaining projects through neighboring PIs, and using calls or new hires to backfill capability where possible (Tables 2.3, 2.4, and 2.8). Another challenge was maintaining coherence while the scientific scope broadened from physics and chemistry into machine learning, open science, metallurgy, and quantum computing. Here the digital infrastructure itself became a coordination device, with AiiDA/AiiDAlab, Materials Cloud, common workflows, RDM strategies and shared tutorials to give heterogeneous groups a practical reason to work within one common ecosystem.

As Materials Cloud, AiiDA and AiiDAlab matured, MARVEL had to combine openness with professionalization. This demanded moderation workflows, scalable backends, legal arrangements, data policies and quality control. The center responded by building a more professional management layer and by connecting itself to external infrastructures such as CSCS, CERN/Invenio, MaX and BIG-MAP. The problem was not removed, but it was transformed from an ad hoc burden on individual laboratories into a collective organizational task.

COVID-19 was an additional stress test. MARVEL shifted reviews, retreats, seminars and strategic meetings online, kept its data-team and governance processes active, and continued fellowships and collaborative events under constrained conditions. The pre-existing habit of structured interaction made this adaptation easier. By the time phase III began, the center was able not only to resume in-person events but also to intensify strategic coordination around legacy and post-2026 planning. That continuity is itself evidence of effective leadership.

Management and leadership performance

The leadership style was pragmatic, adaptive and structurally aware. MARVEL's leadership did not treat the NCCR as a fixed machine. It repeatedly reconfigured the project in response to scientific opportunity, review-panel feedback, budget pressure, personnel changes and the growing importance of digital research infrastructure. Equally important, they were willing to narrow the center when necessary in order to preserve excellence and long-term impact. That choice is especially visible in phase III, where the center accepted a smaller, more focused configuration, and aligned it explicitly with legacy-bearing structures.

For a multi- and interdisciplinary consortium, this is probably the central lesson. Synergy is produced by selectively preserving the forms of breadth that can be made productive. MARVEL's combination of lean central leadership, distributed project ownership, repeated community-building events, selective renewal mechanisms, and a strong common infrastructure was well suited to that task. The management and leadership were one of the main reasons why MARVEL translated a wide Swiss network into durable structural outcomes.

2.5 Conclusion

Structurally, NCCR MARVEL began as a national computational materials network organized around a clear design and discovery pipeline, matured into a set of larger collaborative programs, and ended by deliberately building the institutional and digital structures most likely to survive after the NCCR. Its main achievements are therefore not only organizational descriptions but structural transformations. Experiments were integrated into the heart of the network. Open-science and workflow infrastructures became durable community assets. New hires, chairs and laboratories changed the Swiss institutional landscape. Recurring collaboration formats created a functioning inter-institutional research culture. The legacy is best understood as a distributed national network with durable hubs at PSI, Empa, and EPFL, and with Materials Cloud / AiiDA as its connective digital tissue. The main remaining challenge is to secure the long-term people, governance and service funding needed to run that system after NCCR-specific resources disappear. Yet if that challenge is met, MARVEL's post-NCCR position should remain unusually strong by the standards of time-limited research centers.

3 Scientific impact and international visibility

MARVEL built a recognizable Swiss school of computational materials design and discovery that combined frontier physics, application-oriented materials design, and digital research infrastructure. Scientifically, the NCCR delivered major advances in topological matter, correlated oxides, multiferroics, low-dimensional materials, molecular and nanoporous materials, solid-state ionics, perovskites, and advanced alloys. Methodologically, it created an ecosystem, notably Materials Cloud, AiiDA/AiiDAlab, SIRIUS, and a widening family of machine-learning tools, that turned reproducible high-throughput discovery into a durable capability. The added value of the NCCR resided in the tight coupling of disciplines and institutions: theory with experiment, algorithms with materials applications, and software engineering with scientific discovery. This coupling repeatedly converted isolated scientific ideas into experimentally tested, internationally visible research programs. MARVEL measurably strengthened Switzerland's international position in computational materials science. It did so through high-impact papers, prizes and appointments, European and global partnerships, open-source platforms adopted well beyond the consortium, and, crucially, through structural embedding at PSI and Empa that gives Switzerland a credible path to preserve the standing achieved after the end of the NCCR funding.

3.1 Major scientific contributions — goal attainment and impact

Introduction and overall assessment

NCCR MARVEL began with a dual promise, of predicting and understanding new materials before synthesis, and of making this predictive activity systematic through shared methods, workflows, databases, and theory-experiment feedback loops. The early structure of vertical projects in novel materials physics and applications, supported by horizontal efforts in methods, informatics, and sampling, was already ambitious; over time, the NCCR repeatedly reconfigured itself in order to stay aligned with scientific opportunity and with lessons learned from review panels and internal experience. The resulting trajectory matters for evaluation. Beyond the success of individual subprojects, MARVEL should be judged by the extent to which it transformed materials design and discovery from a set of disconnected expert practices into an interoperable, experimentally anchored, and internationally visible Swiss research capability.

That capability developed in three distinct but continuous waves. In the first wave, MARVEL established scientific credibility through advances in correlated and topological materials, high-throughput screening, and the first version of its open computational infrastructure [1, 2, 3, 4, 5]. In the second wave, the center broadened and sharpened its application portfolio. Low-dimensional materials, molecular crystals, solid-state ion conductors, nanoporous materials, and complex alloys became central, and machine learning moved from a supporting theme to a strategic axis of the NCCR [6, 7, 8, 9, 10, 11, 12, 13]. In the third wave, MARVEL consolidated these achievements into a pillar structure centered on digital infrastructure, atomistic machine learning, spectroscopy, long-term Swiss embedding, and demonstrators that connected simulations directly to experiments and automated platforms [14, 15, 16, 17, 18, 19, 20]. The cumulative result is unusual even by NCCR standards, with a center that contributed scientific concepts, candidate materials, open-source software, FAIR (findable, accessible, interoperable, reusable) data practices, and enduring institutional structures at the same time (Table 3.1).

Phase	Organizational form	Main scientific and methodological emphasis	Representative outcomes
Years 1 to 4	Vertical and horizontal projects; PP7 experimental verification	Correlated oxides, topological materials, energy materials, early machine learning and high-throughput, AiiDA and initial Materials Cloud architecture;	Nickelate low-energy theory; strain rules for titanates/vanadates; disorder-induced multiferroic spirals; β-Bi_4I_4; type-II Weyl semimetals; Z2PACK; first AiiDA release; PP7-funded theory-experiment collaborations.
Years 3 to 4 transition	Reorganisation of VP2 into grand challenges; junior-led collaborative projects after review-panel feedback	Focus on solar cells, water-splitting catalysts, solid-state ionic conductors, low-dimensional materials; new projects in MOFs, catalysts, machine learning, workflows, and structural metals;	Four grand-challenge structures in VP2; recovered CHF 1M for collaborative junior-led projects; new PIs and Agility projects broadened the scientific base.
Years 5 to 8	Design & Discovery and Incubators projects	Molecular crystals, 2D materials, nanoporous materials, complex alloys, oxide heterostructures, scalable ML software and advanced sampling;	2D materials discovery program; quantum spin Hall insulators; solid-state Li-ion conductor screening; librascal/i-PI advances; HEA and alloy-design program; growing Materials Cloud and AiiDAlab ecosystems.
Years 9 to 12	Pillars with explicit digital-infrastructure and long-term-integration missions	FAIR workflows, spectroscopies, exascale readiness, ML for quantum and atomistic observables, direct experiment-simulation integration, Swiss post-NCCR embedding;	Common workflows across 11 engines and 45+ partners; LUMI "hero run"; AIIDAlab experimental interfaces; PSI Laboratory for Materials Simulations; year-11 highlights spanning ML, quantum geometry, spectral methods, and autonomous experimentation.

Table 3.1: *Phase-wise evolution of the NCCR and representative outputs.*

Publications selected by the PIs

In order to provide a bird's eye view on the core accomplishments of the NCCR, we asked all the computational PIs to choose two of their papers that were enabled by MARVEL, together with an explanation for its significance. In addition, we also asked them to point out one paper from other MARVEL groups that they found particularly notable or inspirational. We report this list at the end of this chapter, page 34 — if some PIs are missing, it is because they never replied to our multiple requests.

From condensed matter to predictive discovery

The first phase of MARVEL established a strong scientific identity by attacking problems at the edge of condensed-matter physics while simultaneously developing tools for high-throughput discovery. In correlated oxides, the NCCR solved a long-standing problem in rare-earth nickelates by showing that the metal-insulator transition can be understood in a low-energy e_g description where Mott and Peierls-like physics are intertwined. It changed how the community could think about a canonical class of correlated oxides and led directly to experimental tests via optical spectroscopy and later to systematic studies of the full nickelate series [1, 2, 21, 22]. Closely related work on strain and confinement in early transition-metal perovskites, such as $LaTiO_3$, $LaVO_3$, $CaVO_3$, and heterostructures provided general design rules for how epitaxial strain, surface effects, polarity, and interfaces can drive or suppress metal-insulator transitions. These rules are scientifically valuable because they convert case-by-case calculations into transferable physical guidance for oxide engineering [23, 24].

In magnetism and multiferroics, starting from *ab initio* analysis of $YBaCuFeO_5$, MARVEL identified a new mechanism by which local chemical disorder can generate frustrated bonds in an otherwise unfrustrated lattice, stabilizing polar magnetic spirals at unusually high temperature. Monte Carlo simulations and theoretical analysis established the conditions under which such impurity bonds lead to a spiral rather than to a spin glass, and the idea was then taken forward experimentally toward room-temperature multiferroics [25, 26, 27]. This is a strong example of what the NCCR format can do, by introducing a new physical mechanism, translating it into a design principle, and moving it into the laboratory. The associated work on hexagonal manganites, where the coupled Higgs/Goldstone character of structural modes was identified, similarly connected a deep conceptual question to a concrete material platform [28].

The topological-matter program became one of MARVEL's signature achievements. Already in year 1, the NCCR positioned itself to automate the identification of topological invariants from first principles, a prerequisite for moving from anecdotal discovery to systematic search [29]. This effort rapidly matured into Z2PACK, which provided a universal framework for computing topological invariants from band-structure data and thereby underpinned much of the NCCR's later discovery program [29]. Scientifically, the breakthrough came with the identification of type-II Weyl semimetals and the prediction of materials hosting them, especially WTe_2 and $MoTe_2$, followed by robust candidates, such as MoP_2 and WP_2 [3, 30, 31, 32]. MARVEL also predicted and characterized the strong topological insulator β-Bi_4I_4, nodal-chain metals, triple-point semimetals, and a broader family of candidate topological materials uncovered through large-scale screening [4, 33, 34, 20]. These advances mattered beyond disciplinary prestige because they connected directly to emerging technologies. Realistic tight-binding models for semiconductor nanowires and heterostructures were built to guide the search for Majorana platforms and other quantum-device architectures [35, 36]. More than identifying exotic phases, the topological program engaged with the device-level question of how those phases might be exploited in quantum computing and quantum transport.

Application-driven materials design

In phase I, the goal of the VP2 project was to show that the same predictive culture could be applied to technologically urgent materials domains. In halide perovskites and solar materials, MARVEL groups clarified phase stability, band-gap tuning, carrier localization, temperature-dependent photoluminescence, and the microscopic origin of current-voltage hysteresis [37, 38, 39, 40, 41]. Importantly, this work was carried out in close feedback with leading Swiss experimental groups, especially around perovskite photovoltaics, so that the contribution was design-oriented. Mixed-cation strategies for stability, substitution strategies for band-gap control, and interfaces between absorber and transport layers could be rationalized within a single atomistic framework [37, 39, 40, 41].

In catalysis and energy conversion, MARVEL established descriptors and workflows that turned large, chemically diverse search spaces into tractable discovery problems. The work on oxygen-evolution electrocatalysts and water-splitting catalysts was emblematic. Researchers combined ideas from homogeneous and heterogeneous catalysis, developed volcano-style design relations, and paired these with high-throughput workflows and low-dimensional-material databases to identify plausible catalyst classes [42, 43, 44, 45, 46, 47]. In nanoporous materials and MOFs, the NCCR moved from data curation and property screening toward catalytic mechanism and synthesis optimization, including the use of graph-based matching between structural and isotherm databases and machine-learning assistance for microwave synthesis optimization [48, 49, 50, 51, 52]. These are incremental scientific advances in one sense, but cumulatively they show a rare breadth. MARVEL repeatedly translated state-of-the-art electronic-structure calculations into decision tools for experimental chemistry.

The battery and solid-state-ionics program has a broad impact too. MARVEL created both simplified models and high-throughput pipelines for the identification of solid-state Li-ion conductors, then embedded these in collaborations with PSI and IBM that linked screening, synthesis, electrochemical testing, and improvement cycles [7, 8, 53, 54]. This work had obvious societal relevance in the context of safe, high-performance batteries, but it also had structural significance for the NCCR because it demonstrated the feedback loop between computational filtering and experimental manufacture that the center had promised from the outset. By the later phases, these activities were connected to BIG-MAP and the wider Battery2030+ European effort.

Low-dimensional materials became a second flagship application theme. The high-throughput exfoliation study that identified a large portfolio of two-dimensional materials became one of MARVEL's best-known outputs [6]. Yet the scientific importance lies not only in the celebrated *Nature Nanotechnology* paper [6], but in what followed: mobility workflows, device-level transport simulations with OMEN, screening for quantum spin Hall materials and 2D superconductors (from Jacutingaite [55, 56, 57] to novel magnetism [58]), and collaborations with experimentalists on synthesis, ARPES, and nanoribbon devices [59, 60, 61]. Here MARVEL moved from database creation to full-stack materials design, from atoms and bands to transistors and on-surface molecular electronics.

Later phases extended this application logic to structural metals and advanced alloys. Using machine-learned interatomic potentials, cluster expansion, kinetic Monte Carlo, and discrete-dislocation modeling, the NCCR built a computational metallurgy program capable of addressing natural aging in Al-6xxx alloys, high-entropy-alloy design, Mg plasticity, Cu/W multilayers, Zr hydrides, and aerospace-relevant multi-component alloys [12, 62, 63, 64, 13, 65, 66, 67]. This extension into metals is important strategically, as it was used to enter a domain of direct industrial and societal relevance, including lightweight alloys, refractory alloys, and materials for extreme environments.

Digital infrastructure as scientific contribution

One of MARVEL's most consequential innovations was to treat digital infrastructure as scientific output. The first release of AiiDA in the first phase created an automation, data, environment and sharing framework tailored to computational materials science. Over the following years, this infrastructure was expanded into AiiDA 1.0, a stable workflow engine with provenance, data management, and plugin support for a steadily widening ecosystem of electronic-structure codes [5, 68]. The Materials Cloud developed in parallel as a platform for open computational science, combining an archive with DOIs, curated discover sections, educational material, and later online tools and applications [69]. By 2020, AiiDA was supporting more than 50 simulation packages and Materials Cloud was hosting more than 200 *Archive* submissions and multiple curated datasets, reaching its 1'000th record on 3 April 2024.

The later development of AiiDAlab, Quantum Mobile, common workflows across multiple simulation engines, and robust exascale-ready workflows pushed this contribution even further. AiiDAlab lowered the barrier for non-expert users, including experimentalists, while common workflows and cross-code verification addressed one of the hardest problems in computational materials science: reproducibility across methods, codes, and computing architectures [14, 15, 69].

SIRIUS, DFPT+Hubbard workflows, Koopmans spectral functionals, curated datasets, and the machine-learning software stack (including librascal/rascaline, Q-stack, metatensor and related tools in the later phases) should be understood in the same way. They enabled new science, and became part of the research identity of the NCCR itself. MARVEL was producing software, workflows, and data standards that helped define how modern materials simulations are carried out [70, 71, 16, 17, 72, 10, 11, 73, 74, 19, 75].

Scientific and societal impact

Within the scientific community, MARVEL's impact is visible along four dimensions. First, the center generated discoveries that entered the mainstream literature of condensed-matter and materials science: type-II Weyl semimetals [3], β-Bi_4I_4 [4], two-dimensional exfoliable materials [6], Jacutingaite [55], room-temperature multiferroic design routes [26], machine learning (ML) models for electron density [10] and NMR crystallography [11], common workflows across electronic-structure engines [15], and theory-guided design of BCC high-entropy alloys are all examples [13]. The outcome in term of research outputs is rich. Table 3.2 report 1'420 publications over 12 years, also listed on the website, and these do not count those, which are going out now and in the next months. Review articles are part of the output portfolio of MARVEL, at least 45 of them being identified as such. Another major output of the NCCR are the datasets shared on open repositories, mainly on Materials Cloud *Archive*, and even for part of them on Materials Cloud *Discover*, as curated datasets. MARVEL is thus providing a large number of highly relevant, valuable and impactful datasets. All datasets (about 600) are shared in the dataset index on the MARVEL website. The second dimension of MARVEL impact is its production of open tools, such as Materials Cloud [69], AiiDA/AiiDAlab [5, 68, 14], Quantum Mobile [5], Z2PACK [29], WannierTools [76], HP [17] and Koopmans [77], ShiftML or librascal [73, 78], and others, that expanded the productivity of the broader community. The major codes developed by MARVEL members are listed on the website. Third, the NCCR repeatedly converted methods into validated case studies through the experiments platform PP7 and, later, institutional partnerships, which increased trust in computational design as a scientific practice rather than a purely theoretical aspiration [2, 4, 48, 49, 53]. Fourth, it trained a generation of young researchers to work across physics, chemistry, data science, software engineering, and experimental interfaces.

	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

Table 3.2: *Overview of research outputs (data from: April 2026). The data is self-reported by the NCCR in NIRA and do not count those, which are going out now and in the next months. The numbers of “Review articles” given in the table are a minimal estimate of such kind of publications. In NIRA, they are counted together with the “Research articles in science journals”. The number of datasets in phase I and the first half of phase II are indicative (and a lower limit), as this period was before SNSF policy for datasets.*

The broader societal impact is more indirect. In energy, MARVEL contributed to improved understanding of perovskite photovoltaics [37, 39], water-splitting catalysts [46], solid-state electrolytes [8], battery-characterization workflows [53], and catalytic MOFs and COFs [49, 51], all areas linked to decarbonization and electrification. In digital research practice, it advanced reproducibility, FAIR data, and accessible simulation environments at a time when many scientific fields were struggling with these issues [5, 68, 69, 14, 15]. In technology-facing condensed matter, it provided materials and models relevant to quantum devices, spin transport, and novel electronics [35, 34, 55, 60]. In structural materials, it delivered computational routes toward lighter or higher-temperature alloys relevant to transportation and aerospace [13, 63, 64, 65, 66]. Even where short-term industrial translation was not immediate, the NCCR improved the reliability, speed, and openness of the underlying discovery process, arguably the most durable societal effect that a computation-focused center can have.

Adaptivity

A defining feature of MARVEL was adaptive management, with several explicit reorganizations (see also chapter 2). VP2 was restructured in year 3 into four grand-challenge themes (solar cells, water-splitting catalysts, solid-state ionic conductors, and low-dimensional materials) with some projects merged or discontinued, including the CO_2-capture activity, because concentration of effort promised greater scientific leverage. Following review-panel recommendations, MARVEL recovered CHF 1 million to launch new collaborative projects led by junior or newly arrived personnel, thereby using evaluation feedback strategically. Over time the center moved from the original vertical/horizontal architecture to Design & Discovery projects and finally to a pillar structure that made digital infrastructure, atomistic machine learning, quantum simulations, and long-term Swiss integration explicit strategic goals (Table 3.1).

This adaptation was partly reactive to the rapid evolution of the field. Topological matter exploded internationally during the first years of MARVEL, and the NCCR responded by pivoting from automated invariant calculation to the discovery of new phases, experimentally testable materials, and device-relevant models [3, 29, 4, 30, 31, 20]. Machine learning shifted from an auxiliary approach to a central paradigm in materials modeling, and MARVEL responded by deepening work on representations, uncertainty quantification, density learning, Hamiltonian learning, LLMs, and modular ML software stacks [73, 78, 10, 11, 74, 19, 75]. FAIR data, cloud applications, and exascale readiness likewise became more important internationally over the lifetime of the NCCR. MARVEL often anticipated the changes, particularly through AiiDA, Materials Cloud, SIRIUS, AiiDAlab, and the later integration with electronic lab notebooks and robotic experimentation [5, 68, 69, 14, 15].

At the same time, some ambitions were only partly fulfilled, or were fulfilled later and in a different form than initially envisaged. Already at the end of phase I, some targets remained at the candidate stage rather than at the level of full experimental confirmation. For example Chern-insulator candidates were still expected to be confirmed, the single-band Hubbard material remained a prediction awaiting experimental realization, and the ambition of complete high-throughput characterization of all topological materials in the ICSD had not yet fully crystallized into a public, stable resource on the original timeline. Likewise, the full potential of some application-oriented searches was acknowledged to "still lie ahead" while teams, workflows and datasets were being consolidated. In the applications portfolio, progress was sometimes slower than the early promise because robust discovery workflows, force fields, machine-learning models, and experimental partnerships first had to mature.

These shortfalls reflect the fact that the most ambitious promises of MARVEL involved not only solving known problems, but industrializing the process of discovery itself. Where initial timelines proved optimistic, the NCCR generally reacted productively. It redirected resources toward shared infrastructure, brought in new expertise (for example in structural metals, new machine-learning directions, and later spectroscopy), or changed organizational form so that the most promising lines could scale. In fact, some infrastructure efforts have outperformed the initial plans of the full proposal, especially in informatics and software integration. The center's mature achievement is the creation of an adaptive scientific system capable of preserving momentum while scientific opportunities changed.

3.2 Main scientific value added by the NCCR

The added value of MARVEL collaboration was not incidental. It was designed into the NCCR through institutional diversity (EPFL, ETH Zurich, UniGE, UniBas, UZH, UniFR, USI, PSI, Empa, CSCS, IBM), disciplinary diversity (physics, chemistry, materials science, computer science, mathematics, and engineering), and a formal bridge to experiment through PP7. This architecture mattered scientifically because the central problems of modern materials design and discovery are irreducibly composite. Discovering a new topological phase requires electronic-structure theory, symmetry analysis, numerical implementation, data infrastructure, and experimental spectroscopies. Designing a useful oxide heterostructure requires DFT, many-body theory, strain and defect modeling, growth, and spectroscopy. Building an open workflow that non-experts can trust requires software engineering, HPC know-how, interfaces to multiple simulation engines, and domain scientists who know what counts as a meaningful output. Few groups can do all of this alone and MARVEL repeatedly did it by coordination.

We can see three distinct collaborative mechanisms. The first is deep *theory-theory integration*, combining complementary expertise within computation. The second is *theory-experiment feedback*, using PP7 and later pillar-level partnerships to convert predictions into verifiable projects. The third is *platform collaboration*, using shared infrastructure so that insights from one scientific domain can be reused rapidly in another. Taken together, these mechanisms explain the NCCR's scientific added value (Table 3.3).

Theory-theory integration

Among the clearest examples of added value are collaborations in which one group's scientific problem became another group's methodological breakthrough. The topological-materials effort is the paradigmatic case. The discovery program relied on a close collaboration between Matthias Troyer's and Oleg Yazyev's groups, while Nicola Marzari's group was instrumental for interfacing Z2PACK with Wannier90 and later for integrating topological workflows into the broader open-software ecosystem [29, 3, 32, 30, 5]. This triangle of expertise allowed MARVEL to produce a field-defining tool and a sustainable discovery workflow. The same pattern reappears in the correlated-oxide program. Antoine Georges' many-body expertise and Nicola Spaldin/Claude Ederer's electronic-structure expertise were coupled through the practical need to understand realistic oxides, leading to interfaces between Wannier90 and TRIQS, public software in TRIQS/DFTTools, and validated low-energy descriptions that could be exported across the nickelate and perovskite families [71, 1, 2, 22, 23, 24].

Later phases generalized this logic. Work on molecular materials and atomistic machine learning brought together Ceriotti, Corminboeuf, Goedecker, Parrinello, von Lilienfeld, and later Emsley and Zdeborová in a way that blended sampling, ML representations, uncertainty quantification, and experimental observables such as solid-state NMR [9, 78, 73, 10, 11, 74, 19]. On the metallurgy side, Curtin's work on alloy design and strengthening benefited directly from machine-learning infrastructure and atomistic methods developed in neighbor-

Mechanism	Typical partners	Representative example	Added scientific value
Theory + theory	Electronic structure, many-body theory, symmetry analysis, ML, sampling, device modelling	Troyer-Yazyev-Marzari on Z2Pack and topological workflows; Georges-Spaldin-Ederer on DFT+DMFT/TRIQS; Ceriotti-Corminboeuf-Goedecker on atomistic ML and molecular crystals;	Converts specialized methods into reusable design rules and public software; allows problems to be solved at a scale and reliability unreachable by a single group.
Theory + experiment	MARVEL computational groups with PSI, Empa, UniGE, EPFL experimental teams and external labs	β-Bi$_4$I$_4$ prediction and ARPES confirmation; nickelate optical spectroscopy and later single crystals; multiferroic oxides; solid-state electrolytes and battery materials; Jacutingaite, MOF catalysis;	Raises confidence in predictions, identifies missing physics, and turns computational insight into internationally visible materials discoveries.
Methods + applications	Horizontal/pillar method developers with domain scientists	Hubbard and Koopmans functionals; low-dimensional-material workflows serving photocatalysis, electronics and quantum transport; ML representations serving density, NMR and spectra;	Prevents methods from remaining generic and underused; ensures that new algorithms are shaped by real scientific bottlenecks.
Infrastructure + community	AiiDA/Materials Cloud/AiiDAlab teams, HPC centers, code developers, educators	Common workflows across 11 engines and later 45+ partners; tutorials; Quantum Mobile; ORD integration with ELNs and robotic labs;	Makes the NCCR's scientific practice scalable, reproducible and exportable; amplifies impact far beyond the original projects.

Table 3.3: *Representative collaboration mechanisms and their scientific added value.*

ing MARVEL projects, especially librascal and the broader ML ecosystem [12, 64, 62, 13, 67]. The scientific added value here is "interdisciplinarity" in the sense that it is the conversion of methods into shared research capital. Once developed, these methods could be reused across domains, accelerating later projects and reducing duplication of effort.

Theory-experiment feedback

The experimental-verification platform PP7 was one of the most effective instruments for generating added scientific value. In the first year, PP7 had mainly a networking role and deliberately used calls for proposals rather than pre-allocating funds, so that the center could remain responsive to developments in the theory program and to the capacities of Swiss laboratories. After the 2 calls, in year 2 and then in year 3, 14 new collaborations between computational and experimental partners had been launched. This format mattered because it made experiment a co-designed component of discovery rather than a downstream service. Again, the topological program offers a vivid example. The theoretical prediction of β-Bi$_4$I$_4$ as a new topological insulator was coupled to synthesis at TU Dresden, ARPES at EPFL and Berkeley, transport measurements, and later pressure experiments that revealed superconductivity [4, 79]. The added scientific value was obvious. Experimental anomalies fed back into improved GW calculations, which in turn refined the understanding of the topological phase. This was shared on MARVEL website as one of its success stories, entitled *The search for topological materials in MARVEL: a joint effort of theory and experiment*

The rare-earth-nickelate story is even more exemplary because it unfolded over many years. MARVEL's theoretical description of the insulating state was directly compared with optical spectroscopy from the van der Marel and Triscone groups at UniGE. Later, collaboration with Marisa Medarde's group at PSI led to the growth of single crystals of the wider nickelate family, an advance that had independent international significance and enabled new experimental tests, including Raman evidence for multiferroicity [1, 2, 21, 22]. This is exactly the kind of long-term, cumulative collaborative value a NCCR is supposed to create. Theory identifies the right quantities to measure, experiment provides new sample quality and new constraints, theory adapts, and the field moves.

PP7 also amplified MARVEL's relevance in energy materials. Collaborative projects linked screening and synthesis in solid-state electrolytes, coupled MOF catalyst design to *in situ* characterization, and connected computational spectroscopy with experimental batteries, XPS, XAS and neutron techniques [8, 53, 48, 49, 72, 47]. As the NCCR matured, these collaborations evolved into semipermanent working relations between computational groups and experimental laboratories at PSI and Empa. That transition is itself part of the added value, as it created a shared working culture.

Platform collaboration

A less visible but equally important source of collaborative value came from platform projects and later infrastructure pillars. Materials Cloud, AiiDA/AiiDAlab, Quantum Mobile, and the common-workflows effort allowed groups to exchange not only data but executable research practice. For MARVEL, this meant that a workflow, once developed for one material class or one code, could be turned into a reusable object. There were plugin development across many codes, cross-code verification, high-throughput protocols, graphical interfaces, and online dissemination [5, 68, 69, 14, 15]. These are collaboration enablers in a very concrete sense, as they lower the cost of entering a new domain and increase the return on method development.

This mattered especially once MARVEL diversified. The same infrastructure that served topological screening could support oxide workflows, catalysis screens, spectroscopy calculations, machine-learning datasets, or autonomous battery experiments. The common-workflows project, involving 11 codes and later more than 45 partners worldwide, is perhaps the clearest illustration [15]. Interoperability allowed the center to avoid fragmentation as it expanded scientifically. It also gave MARVEL a collaborative signature that was noticed internationally.

Collaborative breakthroughs

Several collaborations stand out as cases where the added value clearly exceeded the sum of the parts.

Nickelates and oxide heterostructures The integration of low-energy theory, DFT+DMFT, optical spectroscopy, thin-film expertise and later crystal growth yielded a more complete understanding of nickelates than any one component could have produced alone [1, 2, 21, 22, 23, 24]. The same network enabled transfer of insight to titanates, vanadates and later spectroscopy workflows.

Topological materials The combination of theory groups at ETH Zurich and EPFL with ARPES, transport and materials-synthesis collaborators turned abstract topological classification into experimentally recognized discoveries, while tools such as Z2PACK and WannierTools became public goods for the field [29, 3, 4, 32, 30, 31, 33, 34].

Solid-state ionics and batteries EPFL, IBM and PSI formed a particularly effective loop in which screening, approximate ion-transport models, synthesis, testing and refinement fed into each other. We can mention researcher mobility across these institutions and the extension of these activities to external industrial and European partnerships such as Solvay and BIG-MAP [7, 8, 53].

Low-dimensional materials and devices MARVEL's 2D materials portfolio became strategically powerful once paired with transport modeling at ETH Zurich, nanostructure synthesis and characterization at Empa, or synthesis at UniGE. This combination moved the work beyond static databases toward credible device concepts [6, 55, 59, 60].

Autonomous experimentation and open research data The later integration of AiiDAlab with experimental platforms and ELN/LIMS systems, including the year-11 highlight on driving experiments through Empa's Aurora robotic platform, is an excellent example of interdisciplinary added value. It links software engineers, workflow experts, data stewards, experimentalists, and domain scientists in a single research loop [80].

Taken together, these examples show that the NCCR format added scientific value in two ways. It increased the depth of interpretation for specific problems, and it increased the speed with which new methods could propagate across scientific domains.

3.3 International standing — goals, achievements and perspectives

Researcher visibility and reputation

The development of MARVEL's international standing is visible first in the growing recognition of its researchers. Even by the end of phase I, we can mention major individual distinctions. Matthias Troyer received the Aneesur Rahman Prize of the American Physical Society. Nicola Spaldin received the Körber European Science Prize, the L'Oréal-UNESCO

For Women in Science Awards, the Marcel Benoist Prize, the Hamburg Prize for Theoretical Physics. Ursula Röthlisberger, and then Thomas Schulthess received the Doron prize. Michele Parrinello won the Dreyfus Prize. Many MARVEL PIs got ERC grants (24 in total across 3 phases + 3 SNSF ERC "replacement" grants) and all are listed on the website. These distinctions matter because they signal that MARVEL was a host environment for internationally visible leaders.

Yet individual prizes tell only part of the story. The stronger indicator is that MARVEL researchers became associated with identifiable international research agendas: topological matter and topological workflows, correlated oxides and DFT+DMFT, atomistic machine learning, two-dimensional materials discovery, open computational science, and, later, computational spectroscopy and quantum simulations [3, 29, 1, 71, 73, 10, 6, 69, 15, 16, 17]. This thematic visibility persists after the lifetime of any project and attracts collaborators, students, and further funding.

The center's publication profile reinforced this reputation. Across successive phases, publications are recorded in *Nature*, *Science*, *Nature Materials*, *Nature Nanotechnology*, *Nature Communications*, *Physical Review X*, *ACS Central Science*, *npj Computational Materials*, *Energy & Environmental Science*, and other leading venues (e.g., [3, 81, 4, 6, 11, 26, 10, 15, 8]). The point is not simply the number of high-impact papers, but their distribution across subfields. MARVEL achieved international visibility simultaneously in condensed-matter physics, computational chemistry, data infrastructure, machine learning, catalysis, battery materials, and metallurgy. That breadth strengthened the center's reputation as a cross-cutting initiative.

Switzerland's standing in MARVEL research domain

MARVEL advanced Switzerland's international position in several mutually reinforcing ways. It produced scientific results that were globally visible and recognizably Swiss. The topological-materials program linked ETH Zurich and EPFL with Swiss beamline and spectroscopy expertise at PSI, and with Swiss and European university groups, placing Switzerland at the center of a rapidly developing field [3, 4, 30, 31, 33, 34]. The oxide and multiferroic program linked ETH Zurich, UniGE and PSI in a similar way [1, 2, 26], while the perovskite [37], battery and solid-electrolyte [8], 2D-material [6], and alloy programs [13] tied EPFL and Empa/PSI more closely into European application-oriented materials science. In effect, MARVEL made it easier for external partners to see Swiss materials science as a coordinated ecosystem.

The NCCR also created internationally used research infrastructure headquartered in Switzerland. These platforms improved Switzerland's visibility because they were used not only by MARVEL researchers but by a growing external community, supported tutorials and schools, and were integrated into European projects and international collaborations [5, 68, 69, 14, 15]. AiiDA tutorials were held in Trieste, Lausanne, Zurich, Berlin, Accra, Addis Ababa, and Kyoto, with hundreds of participants overall by the end of the early phases, as well as the use of Quantum Mobile to support tens of teaching events with positive feedback [69, 14]. With this international presence, Switzerland was exporting workflows, training environments and standards, in addition to papers.

MARVEL made Switzerland a serious player in open, interoperable, and FAIR computational materials science. There were tight interactions with CSCS, CINECA and Jülich, the MaX and TREX Centers of Excellence, NFFA, BIG-MAP, Marketplace, OpenModel, Dome 4.0, and several other H2020 efforts. Later, the common-workflows verification project involved more than 45 partners worldwide, again with AiiDA playing a central role [15]. This matters strategically because infrastructure is increasingly where scientific influence is exercised. Through MARVEL, Switzerland helped define the way workflows, metadata, provenance, and cross-code validation are organized in materials science.

The NCCR also strengthened Switzerland's position by attracting and retaining early-career talent. We can report a steady stream of postdocs, PhD students, visiting PhD students and master students, new assistant professors, new group leaders, and targeted Agility Plus mechanisms to bring in junior PIs, including women PIs in later phases (Tables 2.2 and 2.5). Review-panel feedback was explicitly used to create junior-led collaborative projects and to broaden the consortium with new expertise in fields such as structural metals, machine learning, and spectroscopy. It is evidence that MARVEL functioned as a talent magnet and career accelerator. The later creation of new permanent or semi-permanent positions at PSI and the long-term role of Empa also show that talent attraction did not end with temporary project funding (Table 3.4).

Dimension	Evidence documented in the reports	Assessment
Scientific recognition	Major individual distinctions for participating researchers, repeated publication in top-tier journals, and global visibility of specific scientific themes such as type-II Weyl semimetals, open workflows, atomistic ML, and 2D materials;	The NCCR raised the international profile of both senior leaders and younger group leaders by linking personal recognition to durable research programs.
Research infrastructure	Materials Cloud, AiiDA/AiiDAlab, Quantum Mobile, common workflows, and curated datasets became internationally used Swiss-led infrastructures;	Switzerland moved from being a contributor to being a convening hub for reproducible computational materials science.
European integration	Work-package roles and partnerships in MaX, TREX, BIG-MAP/Battery 2030+, Marketplace, OpenModel, NFFA, DOME 4.0, Materials Commons, and related activities; collaboration with major European HPC centers;	MARVEL amplified Swiss influence by embedding national expertise in European standards, workflows and training ecosystems. Tight collaboration with CECAM and Psi-k.
Talent and training	International tutorials in Trieste, Lausanne, Zurich, Berlin, Accra, Addis Ababa, and Kyoto; hundreds of tutorial participants; visiting researchers; repeated recruitment of new group leaders, postdocs and PhD students;	The center became a talent attractor and training node, improving Switzerland's visibility among early-career researchers and expert users alike.
Post-NCCR sustainability	Creation of the Division for Scientific Computing, Theory and Data and the Laboratory for Materials Simulations at PSI; support from PSI and Empa, and explicit post-2026 embedding plans;	The NCCR converted temporary project success into institutional capacity, which is the strongest predictor of durable international standing.

Table 3.4: *Selected indicators of the NCCR's international standing and the strengthening of Switzerland's visibility.*

International collaborations and EU integration

MARVEL was deeply embedded in international collaboration networks. Early phase-I projects already collaborated with Microsoft Station Q, Princeton, Yale, Columbia, Lawrence Berkeley National Laboratory, TU Dresden, and other leading groups. As the center evolved, this network expanded to include Cambridge, Stanford, Duke, Aix-Marseille, Regensburg, Parma, Modena, Bremen, Rome, Tokyo, Berkeley and many others, depending on the scientific domain. Such collaborations gave MARVEL access to leading experimental techniques, complementary software ecosystems, and broader benchmark problems.

European integration was particularly strong. MARVEL played work-package roles in the H2020 MaX and TREX Centers of Excellence, NFFA, Marketplace, OpenModel, Dome 4.0, collaborated with Battery 2030+ through BIG-MAP, and helped build standards, metadata and educational resources in partnership with CECAM and other European infrastructures. The NCCR interacted closely with major HPC centers and with European open-data and open-science initiatives, thereby positioning Switzerland as a co-designer of its infrastructures.

This European and international embedding amplified Swiss visibility in a way that individual publications alone could not. It made MARVEL a gateway through which external groups interacted with Swiss laboratories, Swiss software, Swiss HPC resources, and Swiss experimental platforms. That gateway function is one of the clearest markers of international standing.

Early-career researchers

A further, often underestimated, component of international standing is the capacity to attract and socialize the next generation of researchers. Here MARVEL performed strongly. We can report on visiting researchers, including visiting PhD and master students in the early infrastructure phase, and a much broader pattern of attraction through tutorials, software ecosystems, and newly created positions. By year 2 the AiiDA and Materials Cloud activities were already supporting tutorials in Trieste, Lausanne, Zurich, Berlin, Accra, Addis Ababa, and Kyoto, often in partnership with Psi-k, CECAM, ICTP, MaX or local institutions. By year 3 the AiiDA team reported eight tutorials reaching roughly 300 participants, while later phases describe Quantum Mobile being used in tens of events and AiiDAlab lowering the threshold for new users and experimentalists [5, 69, 14]. This training activity is one of the main channels through which a research center becomes globally recognizable.

The NCCR also used organizational renewal as a tool for maintaining scientific relevance and attractiveness. Agility Plus funding and later restructuring rounds brought in or strengthened the roles of junior (and key senior) researchers Ulrich Aschauer, William Curtin, Martin Jaggi, Lyndon Emsley, Ana Akrap, Emiliana Fabbri, Marta Gibert, Sereina Riniker, Zoë Holmes, Michael Herbst, and others across different phases, while phase-III embedding at PSI created visible career paths for Giovanni Pizzi, Michael Schüler, Nicola Colonna, Iurii Timrov and additional postdocs and PhD students (Table 2.5). MARVEL remained porous to new expertise, used evaluation feedback to fund collaborative junior-led projects, and linked recruitment to strategic gaps in the science.

The training effect also reinforced Switzerland's position institutionally. When a tutorial ecosystem, a cloud platform, and a set of high-profile scientific case studies all point to the same national environment, early-career researchers begin to associate that environment with opportunity and credibility. MARVEL achieved this across several communities simultaneously: topological matter, correlated materials, atomistic machine learning, FAIR workflows, catalysis, 2D materials, and computational spectroscopy. In that sense, the NCCR shaped expectations about where cutting-edge computational materials research could be done.

Post-funding prospects and standing

The best evidence that MARVEL's standing can be maintained beyond the NCCR funding period is that the last phase explicitly planned for this question. Pillar 4 was created to support long-term integration into the Swiss scientific landscape, especially through core partnerships with PSI and Empa. The most important institutional development reported is the creation, in 2021, of a new PSI division dedicated to Scientific Computing, Theory and Data, including the Laboratory for Materials Simulations developed in close partnership with MARVEL and headed by Nicola Marzari, with Giovanni Pizzi and Michael Schüler recruited as group leaders, and Nicola Colonna and Iurii Timrov as additional tenure-track scientists, PhD students and postdocs supported or co-supported in that environment. These were supported with cash matching by PSI and Empa, and these structures were explicitly meant to phase in MARVEL's activities beyond 2026.

The standing achieved by MARVEL can be maintained because the NCCR left behind durable assets.

People and positions: international standing is carried by principal investigators, young group leaders, expert scientific software engineers, postdocs and technically skilled experimental collaborators. The creation of permanent or semi-permanent homes for several of these profiles is critical, and MARVEL has clearly advanced in this respect.

Community infrastructure: Materials Cloud, AiiDA/AiiDAlab, Quantum Mobile, common workflows, curated datasets, and the later spectroscopy and ML stacks [5, 68, 69, 14, 15, 10, 11] are not bound to a single grant cycle as long as curation, maintenance and user support continue. Because these infrastructures are already internationally adopted, every year of continued support will yield returns larger than their local cost.

Working partnerships: Collaborations with PSI beamlines, Empa experimental groups, CSCS, European centers, and external code communities are ongoing and increasingly institutionalized rather than project-specific. This network effect is one reason the Swiss position is likely to remain strong.

That said, maintaining the standing is not automatic. The risk is that the shared services which made MARVEL distinctive, workflow maintenance, app development, curation, documentation, tutorials, and the theory-experiment interface, could erode if treated as optional overhead rather than as research infrastructure. Activities, such as documentation days, app support, tutorials, cloud deployment, provenance, and interoperability, require sustained technical staffing and governance. If Switzerland preserves that support, the post-NCCR position is highly promising. If not, MARVEL's most internationally differentiating achievement, its integrated research infrastructure, would be the most vulnerable.

On balance, the prospects are favorable. The center's scientific agenda remains aligned with major international trends: AI-assisted discovery, automated experimentation, reproducible and FAIR research, exascale simulation, quantum materials, batteries, catalysts, advanced alloys, and spectroscopy-informed modeling [73, 10, 15, 3, 8, 13, 17]. Because MARVEL helped shape those trends rather than merely follow them, Switzerland is well placed to remain visible in these domains after the funding period, provided that the institutional structures now in place are allowed to mature.

3.4 The "7 questions"

The review panel asked to deliver an update on the "7 questions" in the final report (*"The '7 questions' defined by the Director for the third phase are praised by the panel. They focus the attention on impact and long-term sustainability for the tools and methods developed in MARVEL in the remaining two years. The review panel looks forward to seeing these questions being brought up again in the final report and at the final event and how they have been addressed"*).

1. Are we discovering novel materials? And interacting with the experimental community on these?
2. Are we pushing machine learning for materials, and making it into a tool for the community?
3. Is AiiDA accelerating or slowing down research? Can it become usable by regular computational scientists?
4. Is the Materials Cloud sustainable? What is it missing and what should be developed/dropped?
5. Are advanced simulation methods accessible and adopted by the community?
6. Is quantum computing going to be viable and useful for materials?
7. Are we missing out on AI and large-language models?

These are sharply the challenges that determine sustainability and impact for MARVEL in the future — these below are the personal answers from the Director:

1. Yes, this is happening and will become ever more a driving force for the future. The community is still beset by inaccurate calculations (e.g., predicting novel materials, that is an extremely tough challenge given the accuracy needed in predicting energetics, and the complexity of phase space and temperature), or by shortcuts in predicting complex properties. So, we believe that our approach (predicting as accurately as possible complex properties, and only for experimentally known materials and structures) is a most promising way forward, and the very accurate verification routes (from pseudopotentals [82, 83] to protocols [84]) will pay dividends for years to come.

2. Yes, and the development of the PET-MAD class of models [85] is testament to the impact of MARVEL for the entire community.

3. This is a difficult answer. I believe that, even after 14 years of development, AiiDA is sparsely used, and the majority of MARVEL PIs (or most researchers worldwide) didn't adopt it. This has definitely had a major negative effect for MARVEL and for all the high-throughput activities — the infrastructure is more comprehensive than anything else available worldwide, but its complexity stops users in their tracks, it distract students from doing research to mastering AiiDA in itself, and it redirected too many resources (from MARVEL to 10+ EU projects) into it. But maybe the development of coding and agentic AI will mean that tools like AiiDA can be extremely precious for their detailed provenance model, and can be managed not by humans, and the deployment of simulation activities through AiiDAlab has been a key success story for MARVEL. Still, this is the only key activity I would not support if I were to go back to 2014 — notwithstanding the amazing quality and care that has gone into it — but it has just stopped too many projects from taking place.

4. Another difficult question. With the exception of CSCS, there haven't been other solutions offered — even the 150K dedicated by EPFL in phase III for Materials Cloud hardware remains unspent thanks to the multiple layers of bureaucracy that make these initiatives stop in their tracks. Very positively, CECAM direct involvement, CSCS identifying materials as one of the two core community to be sustained in the future, CINECA taking over the Materials Cloud *Archive*, strategic alliances with the Science and Technology Facilities Council (STFC), and EU initiatives (from the new EOSC MatOSC node to the Materials Commons) bring hope, but the future remain not as strong, especially for maintaining Swiss ownership.

5. Advanced simulation methods are one of the strengths of the MARVEL community, and the output there was very strong and sustained. The world is instead going into a direction where inexpensive and inaccurate is the norm.

6. Maybe in the future, for strong on-site correlations, it might become useful.

7. We are not missing out, but AI and LLM are going to be revolutionary going forward. MARVEL didn't have the time to build on this, since it's all very recent, but the Jablonka-Smit work [86] was really forward looking in this respect, as is the PET-MAT class of models for machine learning [85].

3.5 Conclusions

NCCR MARVEL should be assessed as a scientific success not only because it discovered or explained important materials phenomena, but because it changed the operating conditions of computational materials research in Switzerland. Scientifically, it delivered high-profile advances in topological matter, correlated oxides, multiferroics, perovskites, low-dimensional materials, molecular and nanoporous materials, solid-state ionics, and complex alloys. Methodologically, it created workflows, software, datasets and open platforms that made these advances reproducible, scalable and exportable. Organizationally, it showed unusual adaptability: it restructured when broader themes were needed, created junior-led projects when reviews demanded sharper collaboration, and responded quickly to new developments in machine learning, digital infrastructures, and automated experimentation. Some specific ambitions remained longer at the candidate stage than initially hoped, especially where experimental realization or full-scale cataloging proved harder than early timelines implied. But the center's response to these gaps was itself a strength: it built the infrastructures and collaborations that make such ambitions progressively more attainable (Table 3.1).

The NCCR's main added scientific value came from its capacity to make collaboration productive rather than ceremonial. Repeatedly, MARVEL connected theory with experiment, methods with applications, and software with scientific discovery in ways that raised the quality and credibility of the resulting science (Table 3.3).

Internationally, the center advanced Switzerland's visibility both through landmark results and through infrastructures — especially AiiDA/AiiDAlab and Materials Cloud — that now shape how researchers inside and outside Switzerland work. With the long-term embedding at PSI and Empa, the standing achieved appears maintainable beyond the end of the NCCR. The broader lesson is that MARVEL did not only discover materials; it discovered an institutional model for doing computational materials science at international level (Table 3.4).

3.6 Practical implications for the post-NCCR period

The evidence in the reports suggests three practical priorities for preserving the standing MARVEL created. The first is to protect the small number of technical activities that produce disproportionately large scientific returns: workflow maintenance, app development, documentation, curated datasets, code interoperability, and user support for non-expert experimentalists. These tasks are easy to underfund because they are not always counted as "scientific" in the narrow sense, yet MARVEL's international visibility rests heavily on them [5, 69, 14, 15]. If Switzerland wants to retain the full value of the NCCR, these functions should be treated as part of the national research infrastructure.

The second priority is to maintain the equivalent of PP7's theory-experiment bridge. One of MARVEL's clearest successes was that computational groups did not operate in isolation from PSI and Empa, nor from university laboratories working on synthesis and advanced characterization. The future Swiss advantage will lie precisely in keeping such feedback loops short. In practical terms, that means preserving flexible seed funding for collaborative projects, continuing to make AiiDAlab and related tools usable by experimentalists, and sustaining the staff positions that can translate between code developers, theorists, and instrument scientists [4, 53, 48, 14].

The third priority is continued renewal. MARVEL remained strong because it repeatedly admitted new expertise — whether in machine learning, spectroscopy, structural metals, quantum simulations, or digital infrastructure. A post-NCCR strategy should therefore avoid freezing the center into a static legacy structure. The more promising route is to preserve the platforms and institutional anchors while leaving room for new principal investigators, junior-led initiatives, and emerging topics. If this balance is maintained, Switzerland will not only preserve the standing achieved during MARVEL; it will continue to set agendas in computational materials design rather than merely participate in them.

3.7 Publications selected by the PIs

12 years of MARVEL through 67 publications

All the computational PIs were asked to choose two of their papers that were enabled by MARVEL, together with an explanation for its significance. This provides a bird's eye view on the core accomplishments of the NCCR.
The publications below are either resulting directly from the NCCR (marked with a red hexagon ⬢) or with minor contributions from the NCCR. All these publications are marked with a green open circle (○), meaning they are accessible in Open Access (OA).

Group of Ulrich Aschauer

⬢○ C. Ricca, I. Timrov, M. Cococcioni, N. Marzari, and U. Aschauer
Self-consistent DFT+U+V study of oxygen vacancies in $SrTiO_3$
Physical Review Research **2**, 023313 (2020).
Group(s): Aschauer, Marzari / Project(s): DD5, DD3

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:sf-4r

We show that the Hubbard U parameter in DFT $+U$, a standard approach for transition-metal oxides, should not be taken as a constant around defects. Computing it self-consistently for different sites, we find U values strongly altered due to the coordination and oxidation state of the transition-metal sites in the vicinity of an oxygen vacancy.

⬢○ C. Ricca, I. Timrov, M. Cococcioni, N. Marzari, and U. Aschauer
Self-consistent site-dependent DFT+U study of stoichiometric and defective $SrMnO_3$
Physical Review B **99**, 094102 (2019).
Group(s): Aschauer, Marzari / Project(s): DD5, DD3

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:nx-r2

We show that not only the on-site Hubbard U parameter but also the inter-site V parameter varies around a defect and show that computing them self-consistently for each site leads to a description of the electronic structure similar to that of much more computationally costly hybrid functionals and in good agreement with experimental measurements.

Group of Sara Bonella

⬢○ F. Angiolari, A. Coretti, M. Salanne, and S. Bonella
Electrically driven first-order phase transition of a 2D ionic crystal at the electrode/electrolyte interface
Proceedings of the National Academy of Science of the USA **122**, e2520026122 (2025).
Group(s): Bonella / Project(s): P3

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:da-za

The arrangement of ions at the interface between a liquid electrolyte and a solid electrode carries key information about important parameters in electrochemical energy storage devices, e.g., super-capacitors. In this paper, we propose an original computational approach, embedding several advanced classical molecular dynamics tools, that reveals a previously undetected two-step interfacial phase transition and asymmetrical patterns at the positive and negative electrode that directly affect the capacitance of the device. These surprising and interesting results are a true MARVEL product, made possible by dedicated Agility funds!

⬢○ D. Du, T. J. Baird, S. Bonella, and G. Pizzi
OSSCAR, an Open Platform for Collaborative Development of Computational Tools for Education in Science
Computer Physics Communications **282**, 108546 (2023).
Group(s): Bonella, Pizzi / Project(s): P3

Links to article: Journal / Open access
Related datasets: doi.org/10.17632/26py5zz9f8.1

This paper presents the OSSCAR open platform for education co-developed by several PIs during the MARVEL project (www.osscar.org). This is a nice example of activities made possible — also — by MARVEL, and in particular by collaborations targeting high-quality training of the community of materials simulators via the creation of a web-based archive of jupyter notebooks. The paper sparked contributions from other PIs, and researchers outside of the project and collaborations to develop bespoke tools (e.g., widgets) to improve the learning experience and increase the flexibility of our toolset.

Group of Giuseppe Carleo

⬢○ D. Wu, R. Rossi, F. Vicentini, N. Astrakhantsev, F. Becca, X. Cao, J. Carrasquilla, F. Ferrari, A. Georges, M. Hibat-Allah, M. Imada, A. M. Läuchli, G. Mazzola, A. Mezzacapo, A. Millis, J. R. Moreno, T. Neupert, Y. Nomura, J. Nys, O. Parcollet, R. Pohle, I. Romero, M. Schmid, J. M. Silvester, S. Sorella, L. F. Tocchio, L. Wang, S. R. White, A. Wietek, Q. Yang, Y. Yang, S. Zhang, and G. Carleo
Variational benchmarks for quantum many-body problems
Science **386**, 296 (2024).
Group(s): Carleo, Georges, Neupert / Project(s): P2, QS

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.8263407

○ J. Nys, G. Pescia, A. Sinibaldi, and G. Carleo
Ab-initio variational wave functions for the time-dependent many-electron Schrödinger equation
Nature Communications **15**, 9404 (2024).
Group(s): Carleo / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.6084/m9.figshare.27102529

The first paper, in *Science*, addressed correlated quantum matter while also clarifying what present and future quantum computers can realistically achieve in this context. The second paper, in *Nature Communication*, introduced a first-principles framework for *ab initio* quantum dynamics based on neural wave functions, opening new possibilities for the study of nonequilibrium many-body systems. Taken together, these papers reflect two central directions of the work: understanding the real scope of quantum computing and developing new tools for quantum dynamics from first principles.

Group of Michele Ceriotti

⬢○ A. Mazitov, F. Bigi, M. Kellner, P. Pegolo, D. Tisi, G. Fraux, S. Pozdnyakov, P. Loche, and M. Ceriotti
PET-MAD as a lightweight universal interatomic potential for advanced materials modeling
Nature Communications **16**, 10653 (2025).
Group(s): Ceriotti / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:fe-1p

This paper is the culmination for MARVEL efforts that are both conceptual (understanding and ultimately overcoming the need for symmetry constraints in atomistic ML models) and infrastructural (implementing a modular ecosystem for training machine-learning models and using them as the engine of simulations). It presents a ML potentials that, thanks to its architecture and a choice of training set based on maximizing the diversity of structures, is fast, stable and accurate across both inorganic and organic materials.

⬢○ A. Grisafi, A. Fabrizio, B. Meyer, D. M. Wilkins, C. Corminboeuf, and M. Ceriotti
Transferable Machine-Learning Model of the Electron Density
ACS Central Science **5**, 57 (2019).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:sw-je

This is one of the first papers demonstrating the use of ML to predict electronic properties, rather than potentials. A collaboration with the group of Clémence Corminboeuf that highlights the collaborative nature of MARVEL, building on the expertise of different groups to realize ambitious projects that would have been very hard to achieve separately.

Group of Volkan Cevher

⬢○ D. E. Carlson, E. Collins, Y.-P. Hsieh, L. Carin, and V. Cevher
Preconditioned Spectral Descent for Deep Learning
in *Advances in Neural Information Processing Systems 28 (NIPS 2015)*, C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, eds. (2015).
Group(s): Cevher, Koch / Project(s): HP5

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

This line of work introduces stochastic spectral descent (SSD), a geometry-aware alternative to coordinate-wise adaptive methods, enabling efficient full-rank updates aligned with modern AI accelerators. It establishes that spectral structure can be exploited at scale and connects naturally to conditional-gradient (Frank-Wolfe) methods, including Muon. Building on this, our recent SCION framework unifies a broad class of optimizers under norm-constrained updates with provable guarantees. Combined with μ-parameterization and μ-transfer, this yields a scale-agnostic training recipe with significant empirical speedups over Adam. This class of algorithms are currently used to train 1 Trillion parameter models.

Group of Clémence Corminboeuf

A. Fabrizio, A. Grisafi, B. Meyer, M. Ceriotti, and C. Corminboeuf
Electron density learning of non-covalent systems
Chemical Science **10**, 9424 (2019).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:v4-xd

Non-covalent interactions govern chemical behavior across scales, yet their accurate characterization remains limited by the cost of computing electron densities. While the total electron density, $\rho(r)$, provides a complete description of bonding and interactions, its evaluation from quantum mechanics is prohibitively expensive for large or high-throughput applications. Here, we introduce a transferable machine learning model that predicts electron densities directly from atomic coordinates, enabling rapid, scalable access to electronic structure information. The model captures both qualitative and quantitative features of non-covalent interactions across diverse systems, from biomolecular fragments to polypeptides. This approach unlocks electron-density-driven analysis at a scale previously inaccessible to quantum chemical methods.

S. Vela, R. Laplaza, Y. Cho, and C. Corminboeuf
cell2mol: encoding chemistry to interpret crystallographic data
npj Computational Materials **8**, 188 (2022).
Group(s): Corminboeuf / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:g5-5r

Crystallographic databases provide vast, chemically diverse, and experimentally validated structures, but lack key information required for quantum chemical computations, such as molecular charges and spin states. To bridge this gap, we introduce cell2mol, a Python package that infers chemically consistent molecular representations from crystal structures, with a focus on transition metal complexes. It automatically retrieves connectivity, charges, bond orders, and oxidation states, converting experimental data into quantum-chemistry-ready inputs. This capability enables scalable, data-driven exploration of transition metal chemistry.

Group of William Curtin

Y. Hu and W. A. Curtin
Modeling of precipitate strengthening with near-chemical accuracy: case study of Al-6xxx alloys
Acta Materialia **237**, 118144 (2022).
Group(s): Curtin / Project(s): P1

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:9m-4n

Y. Rao, C. Baruffi, A. D. Luca, C. Leinenbach, and W. A. Curtin
Theory-guided design of high-strength, high-melting point, ductile, low-density, single-phase BCC high entropy alloys
Acta Materialia **237**, 118132 (2022).
Group(s): Curtin / Project(s): P1

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:a4-yf

In the area of computational metallurgy, we highlight two successes that exemplify the culmination of MARVEL work in bridging of scales from first-principles to quantitative predictions of mechanical properties of alloys. The first work (Hu and Curtin) employs a DFT-trained machine-learning potential developed by our MARVEL team (Curtin and Ceriotti) to directly simulate the strength of the Al-6xxx (Al-Mg-Si) alloy due to the presence of β'' precipitates and thus to guide both calibration of mesoscale discrete dislocation models and validation of theoretical models for precipitate strengthening, reaching good agreement with literature experiments. The second work (Rao *et al.*) identifies new high-temperature refractory bcc high entropy alloys having attractive strength, ductility, and phase stability. Using theories developed by our MARVEL team to search composition space leads to compositions in the Hf-Mo-Nb-Ti-(Ta) family, with $Hf_{15}Mo_{25}Nb_{20}Ta_5Ti_{35}$ and $Hf_{20}Mo_{15}Nb_{30}Ti_{35}$ now fabricated and tested at Empa (group of Leinenbach) and both showing high strength, high melting temperature, with $Hf_{20}Mo_{15}Nb_{30}Ti_{35}$ also having the key performance metric of room temperature tensile ductility (with the groups of Leinenbach and Raju Natarajan).

Group of Claude Ederer

○ A. Carta, I. Timrov, P. Mlkvik, A. Hampel, and C. Ederer
Explicit demonstration of the equivalence between DFT +U and the Hartree-Fock limit of DFT+DMFT
Physical Review Research **7**, 013289 (2025).
Group(s): Ederer, Marzari / Project(s): P4

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:68-g8

This study provides a rigorous and explicit demonstration of the equivalence between DFT +U and the Hartree-Fock limit of DFT + DMFT within a unified Wannier-based framework. By using identical projector functions, it resolves long-standing inconsistencies between the two widely used approaches. Benchmarking across prototypical correlated materials establishes their quantitative agreement and clarifies their theoretical connection. Its methodological unification and broad applicability highlight its importance as a central MARVEL contribution.

○ J. Souto-Casares, N. A. Spaldin, and C. Ederer
Oxygen vacancies in strontium titanate: A DFT+DMFT study
Physical Review Research **3**, 023027 (2021).
Group(s): Ederer, Spaldin / Project(s): DD5

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:jf-zq

This work resolves the long-standing question of the electronic nature of oxygen vacancies in $SrTiO_3$ using a combined DFT+DMFT approach. It demonstrates that the excess electrons can exist in competing localized and delocalized states, governed by electron-electron interactions and lattice geometry. By reconciling previously conflicting experimental and theoretical results, it provides a clear microscopic picture of defect-induced conductivity. This physically transparent and predictive framework makes it a key MARVEL contribution.

Group of Antoine Georges

○ A. Tamai, M. Zingl, E. Rozbicki, E. Cappelli, S. Riccò, A. de la Torre, S. McKeown Walker, F. Y. Bruno, P. D. C. King, W. Meevasana, M. Shi, M. Radović, N. C. Plumb, A. S. Gibbs, A. P. Mackenzie, C. Berthod, H. U. R. Strand, M. Kim, A. Georges, and F. Baumberger
High-Resolution Photoemission on Sr_2RuO_4 Reveals Correlation-Enhanced Effective Spin-Orbit Coupling and Dominantly Local Self-Energies
Physical Review X **9**, 021048 (2019).
Group(s): Georges, Shi / Project(s): DD6

Links to article: Journal / Open access
Related datasets: doi.org/10.17630/592cc7e7-85bb-4bdc-a229-2250bfb728c5

This article brings together theory and experiments in a high resolution angular resolved photoemission (ARPES) study of Sr_2RuO_4, an iconic material which is a model Fermi liquid. The experiments reveal that the effective spin-orbit splitting is enhanced by a factor of 2 as compared to DFT, a theoretical prediction. Importantly, the ARPES results provide a direct validation of the key assumption of dynamical mean-field theory (DMFT), namely that the self-energy has weak angular/momentum dependence when expressed in a basis of local Wannier orbitals.

⬢○ A. Subedi, O. E. Peil, and A. Georges
Low-energy description of the metal-insulator transition in the rare-earth nickelates
Physical Review B **91**, 075128 (2015).
Group(s): Georges / Project(s): VP1

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

This article explains how to understand the remarkable physical properties of the family of transition-metal oxides $RNiO_3$ (R = rare earth) from a low-energy theoretical description that involves only the frontier e_g orbitals. It reveals the crucial role of ligand holes and of the Hund coupling in the observed disproportionation associated with the metal-insulator transition.

Group of Stefan Goedecker

⬢○ D. S. De, M. Krummenacher, B. Schaefer, and S. Goedecker
Finding Reaction Pathways with Optimal Atomic Index Mappings
Physical Review Letters **123**, 206102 (2019).
Group(s): Goedecker / Project(s): DD1

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

This paper describes a method that allows to find complex reaction/transformation pathways where it is initially unknown which atom in the initial structure is mapped onto which atom in the final structure.

⬢○ D. S. De, B. Schaefer, B. von Issendorff, and S. Goedecker
Nonexistence of the decahedral $Si_{20}H_{20}$ cage: Levinthal's paradox revisited
Physical Review B **101**, 214303 (2020).
Group(s): Goedecker / Project(s): DD1

Links to article: Journal / Open access
Related datasets: not applicable

This paper demonstrates that there exist potential energy surfaces whose global minimum is kinetically quasi inaccessible.

Group of Michael Herbst

⬢○ N. F. Schmitz, B. Ploumhans, and M. F. Herbst
Algorithmic differentiation for plane-wave DFT: materials design, error control and learning model parameters
npj Computational Materials **12**, 6 (2026).
Group(s): Herbst / Project(s): P3

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.17084313

This work is the outcome of an interdisciplinary viewpoint on materials simulations, combining advances of mathematical research on response algorithms as well as modern implementation techniques based on the density-functional toolkit. It unlocks novel opportunities for workflows for inverse materials design and error-controlled DFT simulations.

Group of Zoë Holmes

⬢○ M. S. Rudolph, T. Jones, Y. Teng, A. Angrisani, and Z. Holmes
Pauli Propagation: A Computational Framework for Simulating Quantum Systems
arXiv:2505.21606 (2025).
Group(s): Holmes / Project(s): QS

Links to article: Journal / Open access
Related datasets: github.com/MSRudolph/PauliPropagation.jl

This work systematizes Pauli propagation as a practical framework for classically simulating quantum circuits and dynamics, from theory to bit-level implementation. I consider it one of my main MARVEL publications because it turns a promising idea into a usable computational toolbox, including the open-source package PauliPropagation.jl, with clear relevance for quantum simulation and verification. It also has promising longer-term potential for applications in many-body quantum physics and, perhaps eventually, in materials design.

Group of Jürg Hutter

⬢○ A. Bussy and J. Hutter
Efficient and low-scaling linear-response time-dependent density functional theory implementation for core-level spectroscopy of large and periodic systems
Physical Chemistry Chemical Physics **23**, 4736 (2021).
Group(s): Hutter / Project(s): DD4

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:js-me

This paper reports on the implementation of a TDDFT based approach to near-edge XAS spectra for condensed matter systems. Using a core-valence separation and localized orbitals allow for an efficient low scaling treatment of the Sternheimer equations including hybrid functionals.

○ J. Wilhelm, P. Seewald, and D. Golze
Low-Scaling GW with Benchmark Accuracy and Application to Phosphorene Nanosheets
Journal of Chemical Theory and Computation **17**, 1662 (2021).
Group(s): Hutter / Project(s): DD4

Links to article: Journal / Open access
Related datasets: not applicable

This work builds on our implementations of wavefunction correlation methods (MP2, RPA, GW). Previous low-scaling implementations for RPA are here extended for GW. Benchmark calculations are performed to show the accuracy of the method and an application to phosphorene nanosheets highlights its scaling properties.

Group of Christoph Koch

○ A. Shaikhha, Y. Klonatos, and C. Koch
Building Efficient Query Engines in a High-Level Language
ACM Transactions on Database Systems **43**, 4 (2018).
Group(s): Koch / Project(s): HP5

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

⬢○ A. Shaikhha, Y. Klonatos, L. Parreaux, L. Brown, M. Dashti, and C. Koch
How to Architect a Query Compiler
in *Proceedings of the 2016 International Conference on Management of Data* (ACM, New York, NY, USA, 2016), SIGMOD '16, p. 1907.
Group(s): Koch / Project(s): HP5

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

Classical compilers for programming languages such as FORTRAN or C employ only general-purpose optimization techniques that are applicable for all kinds of programs; they cannot leverage knowledge of the application domain (such as materials science). As a consequence, programmers who want to create high-performance code require deep knowledge of the domain, and need to work domain-specific optimizations into the code by hand. These two publications are central to our work on compilers that can automatize domain-specific code optimization. The first won the best paper award at VLDB 2014, the premier international conference on data management.

Group of Teodoro Laino

⬢○ A. Marcolongo, T. Binninger, F. Zipoli, and T. Laino

Simulating diffusion properties of solid-state electrolytes via a neural network potential: Performance and training scheme

ChemSystemsChem **2**, e1900031 (2020).

Group(s): Laino / Project(s): Inc1

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:c3-58

This work was an early and concrete demonstration that neural-network potentials can be used to model ion diffusion in solid-state electrolytes with accuracy close to first-principles methods but at a much more accessible computational cost. It helped connect AI-driven atomistic simulation with a real battery-materials problem and showed a practical route toward faster screening and design of solid electrolytes.

⬢○ T. Binninger, A. Marcolongo, M. Mottet, V. Weber, and T. Laino

Comparison of computational methods for the electrochemical stability window of solid-state electrolyte materials

Journal of Materials Chemistry A **8**, 1347 (2020).

Group(s): Laino, Marzari / Project(s): Inc1

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:rt-ek

This paper provided a systematic comparison of the main computational approaches used to evaluate the electrochemical stability window of solid-state electrolytes. It offered a clear methodological framework for screening and interpreting interface stability in battery materials, which made it especially useful for the broader community working on solid-state batteries.

Group of Mathieu Luisier

⬢○ C. Klinkert, Á. Szabó, C. Stieger, D. Campi, N. Marzari, and M. Luisier

2-D materials for Ultrascaled Field-Effect Transistors: One Hundred Candidates under the Ab Initio Microscope

ACS Nano **14**, 8605 (2020).

Group(s): Luisier, Marzari / Project(s): DD3

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:p8-se

Building on the exploratory work of Mounet *et al.* [6], which revealed 1'825 possibly exfoliable two-dimensional materials, we selected 100 candidates, used them as channel materials of ultra-scaled field-effect transistors (FETs), and simulated their "current vs voltage" characteristics with our in-house quantum transport solver, OMEN. We identified 13 compounds that could deliver performance much larger than conventional, silicon-based FETs, both in an n-type and p-type configuration.

⬢○ A. N. Ziogas, T. Ben-Nun, G. I. Fernández, T. Schneider, M. Luisier, and T. Hoefler

A Data-centric Approach to Extreme-Scale Ab Initio Dissipative Quantum Transport Simulations

in *SC'19: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis* (ACM, New York, USA, 2019), pp. 1:1–1:13.

Group(s): Luisier / Project(s): DD3

Links to article: Journal / Open access

Related datasets: not applicable (before 2020)

In collaboration with the group of Prof. Torsten Hoefler at ETH Zurich, we implemented a new version of OMEN based on a data-centric programming model. The resulting tool, called OMEN-DaCe, was specifically designed to model self-heating effects in realistic field-effect transistors. Running on the Summit supercomputer, OMEN-DaCe reached a sustained FP64 performance of 85 Pflop/s, earning the 2019 ACM Gordon Bell Prize.

Group of Nicola Marzari

⬢○ N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi, and N. Marzari

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

Nature Nanotechnology **13**, 246 (2018).

Group(s): Marzari / Project(s): DD3, OSP

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:jm-zg

This was for us the first work where we did materials discovery, and it was very meaningful materials discovery. The simulations could be trusted, we worked only with experimentally known materials (avoiding the fallacy of trying to predict novel materials, since approximate DFT and the complexity of phase space make these predictions very unreliable). The paper (first on arXiv in 2016) showcased the existence of magnetism in 2D monolayers before it was discovered experimentally, suggested novel classes of 2D materials that had never been explored (e.g., rare-earth trichacogenides), and highlighted novel materials that are now studied extensively (from NiI_2 for magnetism to Nb_3Cl_8 for single band correlations).

○ J. Qiao, G. Pizzi, and N. Marzari
Charting the electronic structure of experimentally known inorganic crystals
under review, Nature Materials and arXiv (2026).
Group(s): Marzari, Pizzi / Project(s): P3, P4

Links to article: not applicable
Related datasets: not applicable

This work, just submitted, does for 3D crystals what the previous one did for 2D monolayers — we explore the entire landscape of known inorganics (excluding lanthanides and actinides, whose complexity still escapes high-throughput explorations), constructing 2 million maximally-localized Wannier functions for 22’000 inorganics, and leading to the discovery of novel thermoelectrics, non-linar Hall effect materials, and 2D electron gas at lattice-matched heterointerfaces.

Group of Titus Neupert

⬢○ S. S. Tsirkin
High performance Wannier interpolation of Berry curvature and related quantities: WannierBerri code
npj Computational Materials **7**, 33 (2021).
Group(s): Neupert / Project(s): DD6

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:1r-8w

We developed the WannierBerri framework to enable highly efficient Wannier interpolation of Berry curvature and related quantities. The work introduced algorithmic advances — including optimized Fourier transforms, symmetry exploitation, and adaptive k-space refinement — that accelerate Brillouin-zone integrations by orders of magnitude. This enables accurate evaluation of transport and topological response properties with extreme accuracy. The open-source implementation provides a flexible platform for future developments in first-principles calculations of electronic and topological phenomena.

○ A. Nelson, T. Neupert, T. Bzdušek, and A. Alexandradinata
Multicellularity of Delicate Topological Insulators
Physical Review Letters **126**, 216404 (2021).
Group(s): Neupert / Project(s): DD6

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:ng-f1

We introduced a new class of topological phases termed delicate topology, where electronic bands appear trivial under standard classifications yet exhibit nontrivial structure because Wannier functions cannot be confined to a single primitive unit cell. By clarifying how topology can persist despite symmetric, localized Wannier representations, it sharpened the conceptual understanding of symmetry-protected band structures and their limitations. The study has influenced ongoing research on delicate and fragile topological phases, guiding both theoretical model building and the search for new topological materials.

Group of Michele Parrinello

⬢○ M. Salvalaglio, C. Perego, F. Giberti, M. Mazzotti, and M. Parrinello
Molecular-dynamics simulations of urea nucleation from aqueous solution
Proceedings of the National Academy of Science of the USA **112**, E6 (2015).
Group(s): Parrinello / Project(s): HP4

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

Group of Daniele Passerone

⬢○ N. Krane, E. Turco, A. Bernhardt, D. Jacob, G. Gandus, D. Passerone, M. Luisier, M. Juríček, R. Fasel, J. Fernández-Rossier, and P. Ruffieux
Exchange Interactions and Intermolecular Hybridization in a Spin-1/2 Nanographene Dimer
Nano Letters **23**, 9353 (2023).

Group(s): Fasel, Luisier, Passerone / Project(s): ASM

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.8128962

In this joint theory/experimental study, it is shown how single-triplet spin excitations in radical nanographenes are dependent on the adsorption substrate (metallic vs insulator). A whole palette of theoretical methods, ranging from extended Hubbard models, through non-equilibrium Green functions, to a multi orbital Anderson model in the one-crossing approximation, allow to disentangle kinetic and Coulomb driven exchange and surface screening, with a quantitative agreement with inelastic tunneling spectroscopy.

G. Gandus, A. Valli, D. Passerone, and R. Stadler
Smart Local Orbitals for Efficient Calculations within Density Functional Theory and Beyond
The Journal of Chemical Physics **153**, 194103 (2020).
Group(s): Passerone / Project(s): DD3

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:33-h8

We present a way to obtain a reduced basis set of atomic orbitals through the subdiagonalization of each atomic block of the Hamiltonian. The resulting local orbitals (LOs) inherit the information of the local crystal field. It is possible to keep only a subset of relevant LOs that provide an accurate description of the physics around the Fermi level. This reduces the redundancy of the original basis set, and at the same time, it allows one to perform post-processing of DFT calculations, ranging from the interpretation of electron transport to extracting effective tight-binding Hamiltonians, very efficiently and without sacrificing the accuracy of the results.

Group of Carlo Pignedoli

A. V. Yakutovich, O. S. Kristjan Eimre, L. Talirz, C. S. Adorf, C. W. Andersen, E. Ditler, D. Du, D. Passerone, B. Smit, N. Marzari, G. Pizzi, and C. A. Pignedoli
AiiDAlab – an ecosystem for developing, executing, and sharing scientific workflows
Computational Materials Science **188**, 110165 (2021).
Group(s): Marzari, Passerone, Pignedoli, Pizzi, Smit / Project(s): DD4, OSP

Links to article: Journal / Open access
Related datasets: github.com/aiidalab/aiidalab-home

I consider this one of the main MARVEL publications from my group because it established the AiiDAlab concept, providing a practical route to make advanced simulation methods more accessible to the broader scientific community. By building on AiiDA, it provides access to robust simulation workflows while naturally supporting reproducibility through full provenance tracking.

A. Kinikar, M. D. Giovannantonio, J. I. Urgel, K. Eimre, Z. Qiu, Y. Gu, E. Jin, A. Narita, X.-Y. Wang, K. Müllen, P. Ruffieux, C. A. Pignedoli, and R. Fasel
On-surface polyarylene synthesis by cycloaromatization of isopropyl substituents
Nature Synthesis **1**, 289 (2022).
Group(s): Fasel, Pignedoli / Project(s): DD3

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:yy-sc

I consider this one a particularly strong MARVEL publication because it shows how advanced DFT simulations can be used effectively in close support of a demanding experimental study of on-surface synthesis. It is also a good example of computational methods becoming accessible enough that an experimentalist could carry out complex simulations with only limited technical input from theory collaborators.

Group of Giovanni Pizzi

E. Bosoni, L. Beal, M. Bercx, P. Blaha, S. Blügel, J. Bröder, M. Callsen, S. Cottenier, A. 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. Kühne, K. Lejaeghere, G. K. H. Madsen, M. Marsman, N. Marzari, G. Michalicek, H. Mirhosseini, T. M. A. Müller, G. Petretto, C. J. Pickard, S. Poncé, G.-M. Rignanese, O. Rubel, T. Ruh, M. Sluydts, D. E. P. Vanpoucke, S. Vijay, M. Wolloch, D. Wortmann, A. V. Yakutovich, J. Yu, A. Zadoks, B. Zhu, and G. Pizzi
How to verify the precision of density-functional-theory implementations via reproducible and universal workflows
Nature Reviews Physics **6**, 45 (2024).
Group(s): Marzari, Pizzi / Project(s): P3, P4

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:s4-3h

In this paper, a systematic and reproducible framework is introduced to assess the precision of density-functional-theory codes, leveraging the AiiDA workflow engine and interoperable AiiDA common workflows to enable cross-code comparisons; it establishes a high-quality reference dataset from two all-electron codes across the whole periodic table, now actively driving improvements in pseudopotential libraries such as SSSP and PseudoDojo, as well as a careful validation of 9 more pseudopotential codes.

X. Wang, E. Bainglass, M. Bonacci, A. Ortega-Guerrero, L. Bastonero, M. Bercx, P. Bonfà, R. De Renzi, D. Du, P. N. O. Gillespie, M. A. Hernández-Bertrán, D. Hollas, S. P. Huber, E. Molinari, I. J. Onuorah, N. Paulish, D. Prezzi, J. Qiao, T. Reents, C. J. Sewell, I. Timrov, A. V. Yakutovich, J. Yu, N. Marzari, C. A. Pignedoli, and G. Pizzi
Making atomistic materials calculations accessible with the AiiDAlab Quantum ESPRESSO app
npj Computational Materials **12**, 72 (2026).
Group(s): Marzari, Pignedoli, Pizzi / Project(s): P3, P4

Links to article: Journal / Open access
Related datasets: github.com/aiidalab/aiidalab-qe, github.com/aiidateam/aiida-quantumespresso

In this paper, the AiiDAlab Quantum ESPRESSO app exemplifies a long-standing MARVEL collaboration by integrating the AiiDA engine, the AiiDAlab platform, and advanced workflows into an accessible situation environment for non-specialists. Simulation workflows have a strong focus on spectroscopy applications relevant to experimental contexts such as Empa and PSI. We deliver a robust, user-friendly platform not limited to single code executions, but executing complete, end-to-end workflow protocols involving even hundreds of simulations.

Group of Anirudh Raju Natarajan

D. K. Lee, Y. L. Müller, and A. Raju Natarajan
Modeling the Equilibrium Vacancy Concentration in Multi-Principal Element Alloys from First-Principles
Acta Materialia **304**, 121752 (2026).
Group(s): Raju Natarajan / Project(s): P1

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:ef-hy

Y. L. Müller and A. Raju Natarajan
Constructing Multicomponent Cluster Expansions with Machine-Learning and Chemical Embedding
npj Computational Materials **11**, 60 (2025).
Group(s): Raju Natarajan / Project(s): P1

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:gn-xa

Research efforts through the NCCR MARVEL have addressed long-standing challenges in alloy theory that have impeded the modeling of finite-temperature thermodynamic and kinetic properties of multicomponent alloys. The embedded cluster expansion is a new formalism that combines machine-learning with chemical embedding schemes to predict atomistic interactions in multicomponent materials from a relatively small pool of electronic structure calculations. This formalism was then leveraged to model point defects in a complex 9-component refractory alloy, capturing how composition and temperature jointly govern defect behavior. Together, these advances enable atomic-scale modeling of high-entropy alloys at experimentally relevant conditions, opening the door to first-principles design of compositionally complex materials.

Group of Volker Roth

V. Nesterov, M. Wieser, and V. Roth
3DMolNet: A Generative Network for Molecular Structures
arXiv:2010.06477 (2020).
Group(s): Roth / Project(s): Inc2

Links to article: Journal / Open access
Related datasets: not applicable

We describe a novel approach to efficiently generate molecular structures that are not restricted to a fixed size or composition. Our model is based on the variational autoencoder which learns a translation-, rotation-, and permutation-invariant low-dimensional representation of molecules. Our experiments yield a mean reconstruction error below 0.05 Å, outperforming the current state-of-the-art methods by a factor of four, and which is even lower than the spatial quantization error of most chemical descriptors.

Group of Ursula Röthlisberger

N. J. Browning, R. Ramakrishnan, O. A. von Lilienfeld, and U. Röthlisberger
Genetic optimization of training sets for improved machine learning models of molecular properties

The Journal of Physical Chemistry Letters **8**, 1351 (2017).

Group(s): Röthlisberger, von Lilienfeld / Project(s): VP2, HP5

Links to article: Journal / Open access

Related datasets: not applicable (before 2020)

⬢○ J. Wiktor, U. Röthlisberger, and A. Pasquarello

Predictive determination of band gaps of inorganic halide perovskites

The Journal of Physical Chemistry Letters **8**, 5507 (2017).

Group(s): Pasquarello, Röthlisberger / Project(s): VP2

Links to article: Journal / Open access

Related datasets: not applicable (before 2020)

Group of Michael Schüler

○ Y. Yen, J. A. Krieger, M. Yao, I. Robredo, K. Manna, Q. Yang, E. C. McFarlane, C. Shekhar, H. Borrmann, S. Stolz, R. Widmer, O. Gröning, V. N. Strocov, S. S. P. Parkin, C. Felser, M. G. Vergniory, M. Schüler, and N. B. M. Schröter

Controllable orbital angular momentum monopoles in chiral topological semimetals

Nature Physics **20**, 1912 (2024).

Group(s): Schüler / Project(s): ASM

Links to article: Journal / Open access

Related datasets: doi.org/10.17617/3.PILCPQ

This work provides the first direct experimental observation, supported by accurate simulations, of orbital angular momentum (OAM) monopoles in chiral semimetals PtGa and PdGa using circular dichroism in ARPES. The advanced modeling of ARPES is the key element for the "smoking gun" signature of the OAM. Our work demonstrates that these OAM textures are robust and can be controlled by reversing the structural handedness (enantiomer) of the crystal, establishing a foundation for future orbitronic device applications.

Group of Thomas Schulthess

⬢○ L. Talirz, S. Kumbhar, E. Passaro, A. V. Yakutovich, V. Granata, F. Gargiulo, M. Borelli, M. Uhrin, S. P. Huber, S. Zoupanos, C. S. Adorf, C. W. Andersen, O. Schütt, C. A. Pignedoli, D. Passerone, J. VandeVondele, T. C. Schulthess, B. Smit, G. Pizzi, and N. Marzari

Materials Cloud, a platform for open computational science

Scientific Data **7**, 299 (2020).

Group(s): Marzari, Passerone, Pignedoli, Pizzi, Smit, Schulthess, VandeVondele / Project(s): DD4, OSP, HPC

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:az-b2; 10.24435/materialscloud:7v-n3

⬢○ S. M. Griffin, P. Staar, T. C. Schulthess, M. Troyer, and N. A. Spaldin

A bespoke single-band Hubbard model material

Physical Review B **93**, 075115 (2016).

Group(s): Schulthess, Spaldin, Troyer / Project(s): VP1

Links to article: Journal / Open access

Related datasets: not applicable (before 2020)

Group of Berend Smit

○ P. G. Boyd, A. Chidambaram, E. García-Díez, C. P. Ireland, T. D. Daff, R. Bounds, A. Gładysiak, P. Schouwink, S. M. Moosavi, M. M. Maroto-Valer, J. A. Reimer, J. A. R. Navarro, T. K. Woo, S. Garcia, K. C. Stylianou, and B. Smit

Data-driven design of metal-organic frameworks for wet flue gas CO_2 capture

Nature **576**, 253 (2019).

Group(s): Smit, Stylianou / Project(s): DD4

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:2018.0016/v3

This work represents one of the first clear demonstrations of AI driven materials design leading all the way from large scale computational screening to the synthesis and experimental validation of a new material that outperformed commercial adsorbents under realistic conditions. By mining more than 300'000 hypothetical MOFs, the study introduced the concept of the "adsorbaphore": a structural motif that optimally binds a target molecule, analogous to the pharmacophore concept in drug discovery. The work showed that AI and molecular simulations can move beyond prediction to uncover transferable physical design principles, enabling the targeted discovery of water tolerant carbon capture materials for industrial flue gases.

⬢○ S. M. Moosavi, A. Nandy, K. M. Jablonka, D. Ongari, J. P. Janet, P. G. Boyd, Y. Lee, B. Smit, and H. Kulik

Understanding the Diversity of the Metal-Organic Framework Ecosystem

Nature Communications **11** (2020).

Group(s): Smit / Project(s): DD4

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:3y-gr

This work introduced a fundamentally new way of thinking about scientific databases: showing that diversity of data can matter far more than sheer size. By quantifying how well a database covers the true chemical design space, the study demonstrated that large but biased datasets can lead to misleading scientific conclusions and poor AI predictions. The work established, for the first time, a rigorous framework to measure novelty and diversity in materials databases, providing a foundation for more reliable AI-driven discovery across chemistry and materials science.

Group of Nicola Spaldin

○ T. N. Tošić, Q. N. Meier, and N. A. Spaldin
Influence of the triangular Mn-O breathing mode on magnetic ordering in multiferroic hexagonal manganites
Physical Review Materials **4**, 033204 (2022).
Group(s): Spaldin / Project(s): DD5

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:qf-c9

This publication provides a comprehensive microscopic understanding of magneto-structural coupling in hexagonal manganites, combining symmetry analysis, model Hamiltonians, and first-principles calculations. It identifies the Mn-O breathing (K1) mode as the key driver controlling magnetic ground states across the series. By linking structural distortions to magnetic interactions, it establishes a predictive framework for tuning magnetism. This integrative, first-principles approach and its clear design implications make it our central MARVEL contribution.

○ V. F. Michel, T. Esswein, and N. A. Spaldin
Interplay between ferroelectricity and metallicity in $BaTiO_3$
Journal of Materials Chemistry C **9**, 8640 (2021).
Group(s): Spaldin / Project(s): DD5

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:f4-94

This work establishes a unified first-principles framework to understand the interplay between ferroelectricity and metallicity in $BaTiO_3$. It disentangles the competing roles of charge carriers, impurity chemistry, and structural distortions in controlling polar behavior. By revealing how doping can both suppress and enhance ferroelectric-like distortions, it provides clear design principles for polar metals. This comprehensive and predictive analysis makes it a key MARVEL contribution.

Group of Ivano Tavernelli

⬢○ M. Rossmannek, F. Pavošević, A. Rubio, and I. Tavernelli
Quantum Embedding Method for the Simulation of Strongly Correlated Systems on Quantum Computers
The Journal of Physical Chemistry Letters **14**, 3491 (2023).
Group(s): Tavernelli / Project(s): QS

Links to article: Journal / Open access
Related datasets: not applicable (no data)

This work extends the reach of quantum computers to realistic materials problems by combining them with classical electronic-structure methods in a quantum-embedding framework. Only the strongly correlated part of a system is treated on a quantum processor, while the rest is handled efficiently on a classical computer. This hybrid strategy reflects MARVEL's core vision: integrating advanced quantum-mechanical models with scalable algorithms to make predictive materials simulations feasible beyond toy systems.

⬢○ S. Piccinelli, A. Baiardi, S. Barison, M. Rossmannek, A. C. Vazquez, F. Tacchino, S. Mensa, E. Altamura, A. Alavi, M. Motta, J. Robledo-Moreno, W. Kirby, K. Sharma, A. Mezzacapo, and I. Tavernelli
Quantum chemistry with provable convergence via randomized sample-based quantum diagonalization
arXiv:2508.02578 (2025).
Group(s): Tavernelli / Project(s): QS

Links to article: Journal / Open access
Related datasets: not applicable (submitted)

This paper presents a new quantum-computing approach that makes it possible to reliably compute molecular energies using realistic, near-term quantum hardware. By combining quantum sampling with robust classical post-processing, the method achieves controlled convergence while significantly reducing hardware demands. This work supports MARVEL's long-term vision of turning quantum simulations into practical tools for predictive materials and molecular design.

Group of Matthias Troyer

⬢○ A. A. Soluyanov, D. Gresch, Z. Wang, Q. Wu, M. Troyer, X. Dai, and B. A.

Bernevig
Type-II Weyl semimetals
Nature **527**, 495 (2015).
Group(s): Soluyanov, Troyer / Project(s): VP1

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

This work predicted a new topological phase of matter — type-II Weyl semimetals — by combining first-principles calculations with symmetry analysis and materials screening. It directly guided subsequent experimental discovery and exemplifies MARVEL's vision of theory-driven materials discovery with strong experimental impact.

⬢○ Q. Wu, S. Zhang, H.-F. Song, M. Troyer, and A. A. Soluyanov
WannierTools: An open-source software package for novel topological materials
Computer Physics Communications **224**, 405 (2018), www.wanniertools.org.
Group(s): Soluyanov, Troyer / Project(s): VP1, DD6

Links to article: Journal / Open access
Related datasets: doi.org/10.17632/ygsmh4hyh6.1

WannierTools provides a high-throughput computational framework to identify and analyze topological materials across broad materials classes. It has become a widely used community standard and reflects MARVEL's impact through shared, open computational infrastructure enabling systematic materials discovery.

Group of Vladyslav Turlo

⬢○ Y. Hu, A. Sharma, G. Lorenzin, J. Yeom, M. Liyanage, W. A. Curtin, L. P. H. Jeurgens, J. Janczak-Rusch, J. Michler, C. Cancellieri, and V. Turlo
Origin of interface stress enhancement and compressive-to-tensile stress transition in immiscible nanomultilayers
Acta Materialia **297**, 121323 (2025).
Group(s): Curtin, Turlo / Project(s): P1

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:8a-gh

This final work in the series explains extreme interface stresses measured in experiments for the immisible Cu/W system by using newly-develop MLIP, reaching quantitative agreement and making predictions for metastable bcc alloy phase formation at the interfaces that was confirmed experimentally with high-resolution electron microscopy. The approach provides a clear pathway for interface stress evaluation and predictive modeling for applications in flexible electronics.

⬢○ S. Gramatte, O. Politano, N. Jakse, C. Cancellieri, I. Utke, L. P. H. Jeurgens, and V. Turlo
Unveiling hydrogen chemical states in supersaturated amorphous alumina via machine learning-driven atomistic modeling
npj Computational Materials **11**, 170 (2025).
Group(s): Turlo / Project(s): P1

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:1p-1m

This work introduces novel approach to modeling H-supersaturated amorphous oxides, enabling characterization of local chemical states in quantitative agreement with experiment. This enables indirect probing of hydrogen chemical state with respect to its composition, critical for predictive design and fabrication of H barrier coatings and nanoporous gas separation membranes.

Group of Anatole von Lilienfeld

○ D. Lemm, G. F. von Rudorff, and O. A. von Lilienfeld
Machine learning based energy-free structure predictions of molecules, transition states, and solids
Nature Communications **12**, 4468 (2021).
Group(s): von Lilienfeld / Project(s): Inc2

Links to article: Journal / Open access
Related datasets: doi.org/10.6084/m9.figshare.c.978904.v5, doi.org/10.24435/materialscloud:53-rw, doi.org/10.24435/materialscloud:sf-tz

Predicting 3D molecular structures conventionally requires costly quantum mechanical energy minimization, limiting exploration of chemical compound space. This work introduced G2S, a machine learning model that infers atomic coordinates directly from a molecular graph, entirely bypassing energy optimization. G2S achieves sub-0.2 Å accuracy across organic molecules, transition states, carbenes, and crystals — on par with or better than established empirical structure generators. Developed during the rise of machine learning for materials within MARVEL, G2S enables scalable structure generation as input for both *ab initio* relaxations and quantum machine learning models.

⬢○ G. F. von Rudorff and O. A. von Lilienfeld
Simplifying inverse materials design problems for fixed lattices with alchemical chirality

Science Advances **7**, eabf1173 (2021).

Group(s): von Lilienfeld / Project(s): Inc2

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.3994178

Searching chemical compound space for new materials is computationally intractable due to its combinatorial scaling — a core challenge addressed within MARVEL, prior to which lead PI Nicola Marzari had already contributed to alchemical approaches. This work reveals a chirality in chemical space arising from the antisymmetry of alchemical nuclear charge perturbations, in analogy to conventional molecular chirality. The resulting “alchemical enantiomers” share identical electronic energies up to third order, reducing the effective dimensionality of chemical space and easing inverse design problems. This symmetry framework provides rigorous, physics-based constraints on chemical bonding that may constrain and complement the data-driven navigation of chemical compound space.

Group of Philipp Werner

⬢○ L. Boehnke, F. Nilsson, F. Aryasetiawan, and P. Werner
When strong correlations become weak: Consistent merging of GW and DMFT
Physical Review B **94**, 201106 (2016).

Group(s): Werner / Project(s): HP3

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

A main MARVEL achievement was the development of the GW + EDMFT approach into a parameter-free *ab initio* framework for correlated electron materials. The first *ab initio* implementation of this scheme, based on a multitier embedding approach, was demonstrated in this paper. This work paved the way for materials simulations with predictive power, and a consistent description of correlations and screening.

○ Y. Murakami, D. Golež, M. Eckstein, and P. Werner
Photoinduced nonequilibrium states in Mott insulators
Reviews of Modern Physics **97**, 035001 (2025).

Group(s): Werner / Project(s): ASM

Links to article: Journal / Open access
Related datasets: not applicable (review article)

On the nonequilibrium side, I would like to highlight our review article on photo-induced states in Mott insulators, which discusses a broad range of phenomena discovered and studied with partial support from MARVEL. Among them is the first nonequilibrium implementation of the GW + EDMFT scheme, which provides the basis for future *ab initio* simulations of photo-excited materials. The review also discusses numerous examples of nonequilibrium design of material properties.

Group of Oleg Yazyev

⬢○ G. Autès, A. Isaeva, L. Moreschini, J. C. Johannsen, A. Pisoni, R. Mori, W. Zhang, T. G. Filatova, A. N. Kuznetsov, L. Forró, W. Van den Broek, Y. Kim, K. S. Kim, A. Lanzara, J. D. Denlinger, E. Rotenberg, A. Bostwick, M. Grioni, and O. V. Yazyev
A novel quasi-one-dimensional topological insulator in bismuth iodide β-Bi_4I_4
Nature Materials **15**, 154 (2016).

Group(s): Yazyev / Project(s): VP1

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

⬢○ G. Autès, D. Gresch, M. Troyer, A. A. Soluyanov, and O. V. Yazyev
Robust Type-II Weyl Semimetal Phase in Transition Metal Diphosphides XP_2 ($X = \mathrm{Mo}, \mathrm{W}$)
Physical Review Letters **117**, 066402 (2016).

Group(s): Soluyanov, Troyer, Yazyev / Project(s): VP1

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

These works identified novel topological materials, specifically the topological insulator β-Bi_4I_4 and the Weyl semimetals MoP_2 and WP_2, via high-throughput screening of the databases of experimentally established crystal structures. Following prompt experimental validation-led entirely by MARVEL researchers in the case of the bismuth halide, these topological materials continue to be actively investigated globally ten years after their discovery.

Group of Lenka Zdeborová

⬢○ L. Clarté, B. Loureiro, F. Krzakala, and L. Zdeborová
On double-descent in uncertainty quantification in overparametrized models
in *Proceedings of The 26th International Conference on Artificial Intelligence and Statistics*, F. Ruiz, J. Dy, and J.-W. van de Meent, eds. (PMLR, 2023), vol. 206 of *Proceedings of Machine Learning Research*, pp. 7089–7125.

Group(s): Zdeborová / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:zb-71

This paper extends the analysis of uncertainty to more realistic learning scenarios, closer to those encountered in materials modeling. It probes how standard uncertainty quantification methods perform in high-dimensional overparameterized settings, identifying when they are reliable and when they fail to provide accurate uncertainty estimates. I view it as central because it contributes to a principled understanding of reliability in modern data-driven approaches.

Emblematic publications

In addition, we asked the computational PIs to choose one emblematic MARVEL publication outside their group. The two first (Mounet *et al.* and Mazitov *et al.*) were the ones mentioned more often.

N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi, and N. Marzari
Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds
Nature Nanotechnology **13**, 246 (2018).
Group(s): Marzari / Project(s): DD3, OSP

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:jm-zg

The universe of two-dimensional materials beyond graphene holds enormous promise, yet only a handful had been experimentally realized due to the lack of a systematic strategy for identifying viable candidates. This work used AiiDA-automated density functional theory calculations — including van der Waals corrections and random-phase approximation binding energies — to screen 108’000 known three-dimensional compounds and identify nearly 2’000 that are easily or potentially exfoliable. For a subset of 258 materials, electronic, vibrational, magnetic and topological properties were computed, uncovering 56 magnetic systems and multiple topological candidates, demonstrating the power of DFT-based high-throughput approaches to narrow vast chemical spaces down to actionable targets. By making all data and full calculation provenance openly available through the Materials Cloud, the work established a community resource that continues to guide experimental synthesis efforts worldwide.

A. Mazitov, F. Bigi, M. Kellner, P. Pegolo, D. Tisi, G. Fraux, S. Pozdnyakov, P. Loche, and M. Ceriotti
PET-MAD as a lightweight universal interatomic potential for advanced materials modeling
Nature Communications **16**, 10653 (2025).
Group(s): Ceriotti / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:fe-1p

This is an emblematic publication because it provides a reusable model for atomistic materials chemistry and is expected to have an impact well beyond a single code, workflow, or class of materials. The work enables the lineup of next-generation foundational potentials for materials research across periodic table of elements.

K. M. Jablonka, P. Schwaller, A. Ortega-Guerrero, and B. Smit
Leveraging large language models for predictive chemistry
Nature Machine Intelligence **6**, 161 (2024).
Group(s): Smit / Project(s): P1

Links to article: Journal / Open access
Related datasets: github.com/kjappelbaum/gptchem

This paper was really forward-looking at seeing the power of large language models in science.

C. Ricca, I. Timrov, M. Cococcioni, N. Marzari, and U. Aschauer
Self-consistent DFT+U+V study of oxygen vacancies in $SrTiO_3$
Physical Review Research **2**, 023313 (2020).
Group(s): Aschauer, Marzari / Project(s): DD5, DD3

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:sf-4r

S. P. Huber, S. Zoupanos, M. Uhrin, L. Talirz, L. Kahle, R. Häuselmann, D. Gresch, T. Müller, A. V. Yakutovich, C. W. Andersen, F. F. Ramirez, C. S. Adorf, F. Gargiulo, S. Kumbhar, E. Passaro, C. Johnston, A. Merkys, A. Cepellotti, N. Mounet, N. Marzari, B. Kozinsky, and G. Pizzi
AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance
Scientific Data **7**, 300 (2020).
Group(s): Marzari, Pizzi / Project(s): DD3, OSP

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:st-ht; 10.24435/materialscloud:az-b2

⬢○ G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, and B. Kozinsky
AiiDA: automated interactive infrastructure and database for computational science
Computational Materials Science **111**, 218 (2016).
Group(s): Marzari / Project(s): PP6

Links to article: Journal / Open access
Related datasets: not applicable (no data)

⬢○ L. Talirz, S. Kumbhar, E. Passaro, A. V. Yakutovich, V. Granata, F. Gargiulo, M. Borelli, M. Uhrin, S. P. Huber, S. Zoupanos, C. S. Adorf, C. W. Andersen, O. Schütt, C. A. Pignedoli, D. Passerone, J. VandeVondele, T. C. Schulthess, B. Smit, G. Pizzi, and N. Marzari
Materials Cloud, a platform for open computational science
Scientific Data **7**, 299 (2020).
Group(s): Marzari, Passerone, Pignedoli, Pizzi, Schulthess, Smit, VandeVondele / Project(s): DD4, OSP, HPC

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:az-b2; 10.24435/materialscloud:7v-n3

⬢○ M. Ceriotti
Beyond Potentials: Integrated Machine Learning Models for Materials
MRS Bulletin **47** (2022).
Group(s): Ceriotti / Project(s): P2

Links to article: Journal / Open access
Related datasets: not applicable (review article)

The integration of machine learning and artificial intelligence in the discovery of new materials and, in general, is perhaps the most interesting revolution that occurred — or at least accelerated dramatically — during the MARVEL funding period. This is a great review from one of the leaders in the field, and a key member of NCCR, that showcases the broad range of applications of ML: from the delivery of accurate interactions to the calculation of non-trivial functional properties of condensed phase systems. While a new version might have to be written soon — a testament to the progress in the domain, to which MARVEL has substantially contributed — this is a rich and clear starting point of any practitioner.

⬢○ F. Musil, A. Grisafi, A. P. Bartók, C. Ortner, G. Csányi, and M. Ceriotti
Physics-Inspired Structural Representations for Molecules and Materials
Chemical Reviews **121**, 9759 (2021).
Group(s): Ceriotti / Project(s): DD1

Links to article: Journal / Open access
Related datasets: not applicable (review article)

This as an emblematic MARVEL publication because it captures one of the project's most influential themes: bringing machine learning and atomistic modeling together in a rigorous, physically grounded way. It has also become a widely recognized reference for structural representations in materials and molecular machine learning.

⬢○ F. Musil, M. J. Willatt, M. A. Langovoy, and M. Ceriotti
Fast and Accurate Uncertainty Estimation in Chemical Machine Learning
Journal of Chemical Theory and Computation **15**, 906 (2019).
Group(s): Ceriotti, Jaggi / Project(s): DD2

Links to article: Journal / Open access
Related datasets: not applicable (no data)

⬢○ A. Marrazzo, M. Gibertini, D. Campi, N. Mounet, and N. Marzari
Relative Abundance of $\mathbb{Z}_2$ Topological Order in Exfoliable Two-Dimensional Insulators
Nano Letters **19**, 8431 (2019).
Group(s): Marzari / Project(s): DD3

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:4p-q2

⬢○ A. Cepellotti and N. Marzari
Thermal Transport in Crystals as a Kinetic Theory of Relaxons
Physical Review X **6**, 041013 (2016).
Group(s): Marzari / Project(s): VP2

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

⬢○ S. Gramatte, O. Politano, N. Jakse, C. Cancellieri, I. Utke, L. P. H. Jeurgens, and V. Turlo
Unveiling hydrogen chemical states in supersaturated amorphous alumina via machine learning-driven atomistic modeling
npj Computational Materials **11**, 170 (2025).
Group(s): Turlo / Project(s): P1

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:1p-1m

⬢○ Y. Rao, C. Baruffi, A. D. Luca, C. Leinenbach, and W. A. Curtin
Theory-guided design of high-strength, high-melting point, ductile, low-density, single-phase BCC high entropy alloys
Acta Materialia **237**, 118132 (2022).
Group(s): Curtin / Project(s): P1

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:a4-yf

○ N. L. Nguyen, N. Colonna, A. Ferretti, and N. Marzari
Koopmans-Compliant Spectral Functionals for Extended Systems
Physical Review X **8**, 021051 (2018).
Group(s): Marzari / Project(s): HP3

Links to article: Journal / Open access
Related datasets: not applicable (before 2020)

4 Knowledge and technology transfer

4.1 Strategies, aims and resources

The NCCR MARVEL's vision for knowledge and technology transfer (KTT) centers on the development and dissemination of open-source materials simulation codes, the training of users in advanced computational methods, the deployment of the materials informatics framework (AiiDA), the open sharing of curated and raw data with provenance via the Materials Cloud, the strengthening of verification and validation, and the connection of these capabilities to experimental and industrial users. Knowledge transfer targets traditional academic computational groups, but also reaches out to experimental groups and industrial researchers. Technology transfer aims to engage the industrial community that can benefit from simulation tools, fostering research collaborations locally and globally.

Phase I concentrated on community formation and infrastructure building. Phase II turned AiiDA and the Materials Cloud into operational user facilities (AiiDAlab was created) and aligned specific Design and Discovery (D&D) research projects with five key industrial sectors: materials for energy, materials for electronics, pharma & fine chemistry, chemistry & catalysis, and metals. Phase III focused on the long-term sustainability of these platforms, standardized interfaces, cloud and on-premise deployment, digital education, and actively embedding MARVEL tools in public and private institutions.

Resource allocation for KTT scaled and adapted with the project's maturity. In phase I, a dedicated industrial liaison officer was hired at 0.20 FTE. In phase II, an additional 0.15–0.20 FTE was allocated for a scientific writer to boost industrial communication, write feature stories, and manage social media. Initial interactions revealed that small and medium enterprises (SMEs) were not aware of the field of quantum simulations and often didn't understand what to expect. Consequently, MARVEL proactively pivoted its technology transfer focus toward large companies (e.g., Solvay, Microsoft, Bosch, Samsung) that already possessed internal R&D capabilities. To formalize this engagement, MARVEL created an Industrial Advisory Board (IAB) and launched targeted "Industry Sector Days" to systematically capture the pre-competitive needs of these major players. In phase III, the budget line became smaller because major platform work was increasingly carried by the Open Digital Infrastructure pillar and external projects, while TT efforts narrowed toward deployable AiiDAlab instances, industry-embedded postdocs, and long-term stewardship.

4.2 Highlights and overall impact

The overall impact was strongest on the knowledge-transfer side. MARVEL created a globally visible open-science ecosystem around AiiDA/AiiDAlab, Materials Cloud, and Quantum Mobile. From the first open-source AiiDA release in 2015, the platform evolved into a broad community infrastructure: in 2026, the AiiDA registry counts 105 plugin packages supporting 180 simulation codes and more than 200 workflows, with many maintained outside MARVEL. This external uptake is a strong indicator of genuine community transfer rather than simple project-internal usage. The Materials Cloud and in particular its *Archive* followed a similar path: first beta-released in 2017, re-engineered in 2020 around CERN technology, then recognized by *Nature*'s *Scientific Data*, *Open Research Europe* and the SNSF as a recommended repository for materials-science data. Quantum Mobile and repeated international tutorials extended these assets into teaching, reproducible workflows and on-boarding at scale.

MARVEL firmly established its software infrastructure at the heart of the European materials modeling ecosystem. The NCCR successfully leveraged its tools to secure roles in

Figure 4.1: Plenary talk by Lucia Reining at the Psi-k 2022 conference in Lausanne.

massive European H2020 projects, including the MaX Centre of Excellence, MarketPlace, INTERSECT, EMMC, and the BIG-MAP battery initiative, as well as Swiss initiatives, such as SwissTwins and PREMISE. A particularly convincing translational example came from Empa, where tailored AiiDAlab applications let experimentalists browse, launch and analyze workflows themselves, shifting the interaction with modelers away from technical setup and toward scientific interpretation. The review panel explicitly highlighted the securing of the long-term fate of data and open-science software at PSI as a major achievement, noting that this is where many comparable projects fail. A crowning achievement in community engagement was the organization of the Psi-k 2022 conference at EPFL, which became the largest worldwide event in electronic structure, gathering 1'260 participants (Fig. 4.1). This was repeated with the 2025 edition also organized at EPFL with over 1'300 participants.

Regarding technology transfer, contacts with the industrial community were reinforced with the setup of an Industrial Advisory Board representing the 5 industrial sectors covered by MARVEL research (metals, chemicals, ICT, energy, pharma). The "Industry Sector Days" related to the same topics proved to be a highly successful format for bridging academia and industry, resulting in actionable feedback that directly influenced research directions. Collaborations were set with major companies such as Solvay, Samsung, Bosch, Gaznat, Microsoft, BASF and Materials Design, with almost CHF 7 millions in funding. The 2024 Empa Industry Day, with about 100 participants and speakers from IBM, BASF, Bosch, Microsoft, Schott and Beyond Gravity, showed that MARVEL had become a credible convening platform for academic-industrial dialogue.

As also visible in Table 4.2, MARVEL privileged open-source dissemination, shared infrastructures and collaborative R&D more than classic licensing or spin-off creation; as a result, value was captured mainly through open platforms, demonstrators, contracts, public-private projects and the movement of trained people into industry. The less successful side of the portfolio lies exactly there: direct uptake of MARVEL software in companies remained harder than expected, unless they already had computational materials and Python expertise. As explicitly noted by the review panel, one of the most effective modes of technology transfer occurs when companies hire trained MARVEL researchers. Fig. 4.3 (left) illustrates that 57 junior researchers (16%) transitioned to the private sector and 6 (2%) to the public sector, just after their time in MARVEL. Moreover, if we consider the present employer (as of spring 2026) of MARVEL PhD students and postdocs, the proportion grows up to 40% to the private sector, with still 2% to the public sector (Fig. 4.3, right). This flow of highly skilled personnel into industry — including notable placements at Schott (Leopold Talirz), BASF (Sandip De), Stellantis

	Innosuisse projects	**Patents**		**Licenses**	**Prototypes / Demonstrators**	**Start-ups / spin-offs**	**Other (NDA)**
Phase I	2	5	(3 granted)	1	3	0	6
Phase II	0	3	(0 granted, 1 pending)	0	4	0	3
Phase III	2	2	(2 pending)	0	1	0	0
Total	4	10	(3 granted)	1	8	0	9

Table 4.2: Output knowledge and technology transfer (data from: April 2026). The generation of 10 patents and 8 prototypes/demonstrators underscores the practical relevance of the NCCR's discoveries. The 9 NDAs emphasize the active and confidential discussions maintained with numerous large companies to establish collaborative research frameworks. Although no start-ups/spin-offs are reported in the table, a start-up pathway is currently being explored by Giovanni Pizzi and Carlo Pignedoli through an SNSF BRIDGE discovery proposal focused on translating MARVEL-developed workflow and platform technologies into a sustainable service model.

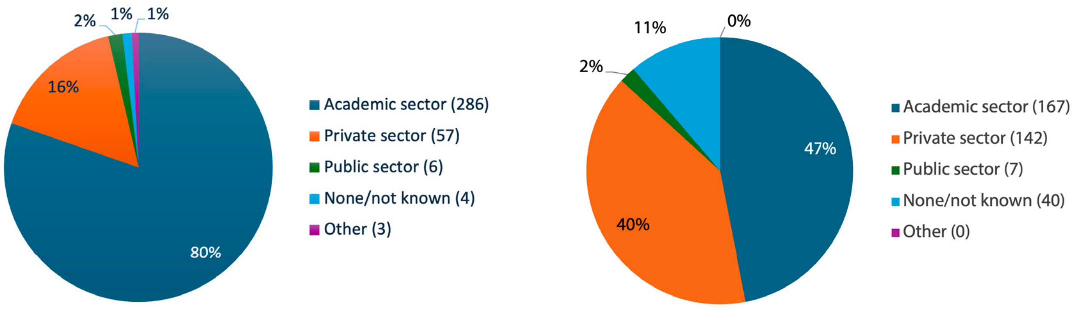

Figure 4.3: *Next employment of PhD students and postdocs after finishing their work in the NCCR (left), and current employment in spring 2026 (right).*

(Giulia Mangione), Dow (Chiara Ricca), Materials Design (Leonid Kahle, Michele Kotiuga), and NVIDIA (Simon Adorf), as shared through portraits of alumni who moved to industry — serves as the primary conduit for embedding complex computational modeling skills into the industrial R&D ecosystem. To prepare them, MARVEL actively organized round tables, IP rights training, and interactions with the Industrial Advisory Board during junior retreats and MARVEL review and retreats. We can specifically mention the 2023 junior retreat on "Building bridges".

4.3 Experiences and outlook

MARVEL will leave a profound and enduring legacy beyond its funding period. The Materials Cloud *Archive* is now a fully established, long-term open-access repository officially recommended by the SNSF, *Nature*'s *Scientific Data*, and *Open Research Europe*. The AiiDA platform and the Materials Cloud have become the backbone for numerous European computing initiatives, ensuring its sustained development and maintenance through external consortia like BIG-MAP and SwissTwins. AiiDAlab offers tailored applications for experimentalists and common standards such as OPTIMADE and reusable workflow interfaces are made available. Furthermore, educational resources such as the digital platform OSSCAR (developed with EPFL and CECAM) and the open-source Quantum Mobile will continue to serve global classrooms. In April 2026, a CECAM-PSI Collaboration Agreement is about to be signed with the objective to organize an annual joint workshop on a topic that aligns with the scientific interests of both institutions. Most importantly, the human legacy of researchers who carry MARVEL's methodologies into the private and public sectors will permanently elevate the landscape of computational materials design.

Collaboration with home institutions and service units was foundational to MARVEL's success. The NCCR relied heavily on the Swiss National Supercomputing Centre (CSCS) for hardware infrastructure and the robust hosting of the Materials Cloud. The KTT team worked in deep synergy with EPFL's Technology Transfer Office (TTO), the Alliance industrial liaison program, and various EPFL Centers to successfully pinpoint and approach target companies. Additionally, collaborations with former CCMX and the Empa Akademie were particularly useful for industry-facing events, such as workshops or a highly successful Industry Day that facilitated direct dialogue with industrial partners.

The legacy phase offers a strong opportunity to consolidate MARVEL outputs into robust, usable and sustainable tools. Industry repeatedly asked for user-friendly interfaces, long-term support, compatibility with existing IT environments, and workflows that bridge atomistic simulation to manufacturing, defects, and device or process performance. MARVEL has already addressed part of this need through AiiDAlab apps, standardized APIs, common workflow interfaces, custom deployment scripts, and sector-specific collaborations. The integration of machine-learning tools developed within MARVEL, such as the QML toolkit, chemiscope, and metatensor, further strengthens this direction and is already being deployed to tackle complex industrial challenges. The most realistic post-NCCR model is therefore a mixed one: openly maintained community tools, institutional stewardship for archives and services, and selective deeper embedding in companies or public labs when a clear use case and support model exist.

5 Education and training

5.1 Strategies, aims and resources

Across the funding period, MARVEL treated education and training as a mechanism for community formation, skills transfer and long-term field building: first by mapping and connecting existing courses, then by empowering junior researchers to organize schools and retreats, and finally by turning successful training events into durable digital and institutional assets. The primary aim was to train a new generation of computational materials scientists able to work across physics, chemistry, materials science and computer science and to increase the interest of youth in science, technology, engineering, and mathematics (STEM) fields.

In phase I, the strategy was deliberately foundational. MARVEL first identified the relevant Master- and PhD-level offerings across the participating institutions, then sought to connect them through a common doctoral-school vision, tele-teaching, yearly junior retreats, support for external schools and workshops, and the first idea of an education platform with recorded lectures and reusable learning material. The evaluation of phase I led to a major strategic adaptation. The reports explicitly note that a coherent cross-university training programme proved harder to implement than expected, even though the individual classes and activities were considered high quality. In phase II, MARVEL therefore shifted from trying to impose a single common curriculum to a more flexible model. Existing local offers were curated and adapted for the community; student-led retreats, junior seminars and summer schools became central. The proposed MARVEL Academy and EPFL minor in computational materials design were explored; discussions revealed though that implementing a cross-departmental curriculum interfered too much with existing semester-long classes. Consequently, MARVEL adapted its strategy to focus heavily on digital education, MOOCs, the education platform, using Materials Cloud *Learn* and Quantum Mobile. In phase III, this logic was pushed further. Education adapted toward a robust digital education platform providing open-access interactive tools, supported by the dedicated OSSCAR initiative, advanced online courses, the Lhumos platform, aiming to leave a lasting impact beyond the end of the NCCR.

5.2 Highlights and overall impact

The most successful measures were the ones that gave junior researchers both ownership and visibility. The main example was the annual Junior Retreats, entirely organized by and for PhD students and postdocs. These 3-to-4-day events fostered creative collaboration by actively grouping 35 to 50 young researchers from different institutions to brainstorm and pitch independent research projects, directly nucleating original research within the NCCR (Fig. 5.1). Furthermore, MARVEL supported highly successful student-organized summer schools, such as the 2019 "Advanced Electronic Structure Methods in Condensed Matter Physics", which attracted 146 international participants, including 53 current MARVEL members. After the pandemic, the junior retreat resumed in 2023 and 2024, with about 60 participants each. These events mattered not only because of attendance, but because

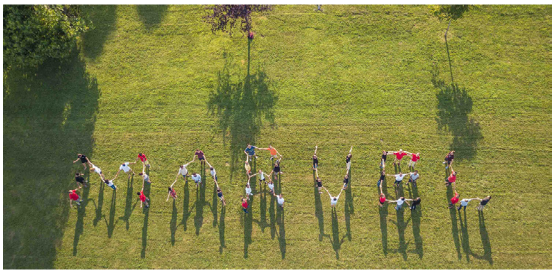

Figure 5.1: *Group photo at the third MARVEL junior retreat on 3—7 July 2017 in Magliaso, Ticino. Picture: Sandip De, NCCR MARVEL.*

they trained junior scientists in organization, public speaking, community building, and agenda setting. In the same line, the junior seminars, held on a monthly basis and organized by a junior committee, aimed to intensify interactions between the MARVEL junior scientists belonging to different research groups, with regularly a participation of 40 to 60 people on site and 10-20 online.

MARVEL's impact on training programs was also realized, enhanced, and made durable through its digital education platforms. The NCCR successfully developed and deployed tools like the Materials Cloud *Learn* platform and recorded lecture series — such as the MARVEL Distinguished Lectures and the highly successful CECAM-MARVEL Classics in molecular and materials modeling; Quantum Mobile as a uniform software environment for teaching, with interactive Jupyter notebooks and virtual machines; OSSCAR (Open Software Services for Classrooms and Research) notebooks used in Bachelor and Master courses; and later the Lhumos portal as successor to Materials Cloud *Learn*; all these providing open-source educational infrastructure that is globally accessible. MARVEL also extended its educational impact internationally by actively co-sponsoring and providing mentors for the African School on Electronic Structure Methods and Applications (ASESMA) (Fig. 5.2), supporting the ASESMAnet network and the EPFL Excellence in Africa (EXAF)-linked Kigali activities, and funding a 2-year Master's fellowship at ICTP-East African Institute for Fundamental Research (ICTP-EAIFR), at the University of Rwanda, providing research exposure for African students and early-career researchers.

For the younger generation, a particularly successful measure was the launch of the summer camp for high school students *Des atomes aux ordinateurs, à la découverte de la programmation scientifique*. First held in 2018, this camp introduced high school students to Python programming, cellular automatons, molecular dynamics, and machine learning, reserving half the seats for young women (Fig. 5.3). The camp consistently received overwhelmingly positive student evaluations, successfully inspiring youth to explore computational materials science. The activity, developed in collaboration with the EPFL Education Outreach Department, will continue, in 2026 as *Matériaux : innover à l'échelle atomique*, under the supervision of MARVEL PI Anirudh Raju Natarajan.

Figure 5.2: ASESMA school in Kigali, Rwanda, on 12-23 June 2023. ASESMA aims to introduce young African researchers to the theory of electronic structure. Picture: Iurii Timrov, NCCR MARVEL.

Figure 5.3: Summer camp for high school students, edition 2025, 23–27 June at EPFL.

MARVEL trained 209 PhD students and 239 postdocs, and this educational effort was central throughout the phases, with PhD students recruitment remaining strong into phase III, when funding was reduced (Table 5.4), and still an important group of postdocs in this last phase. The impact of this training and career development is evidenced in Fig. 4.3, which shows an 80% retention rate in the academic sector as direct next employment (left panel), and still 47% in spring 2026 (right panel). This difference is due to the fact that many students are continuing with a postdoc after their PhD, or a even second postdoc, before leaving academia to the private or the public sectors. In any case, this highlights MARVEL's profound success in nurturing scientific excellence and preparing young scientists for highly competitive academic careers. The 16% (next employment) to 40% (spring 2026) transition into the private sector is also worth noting and is commented in chapter 4 on

	Phase I	Phase II	Phase III	All phases
PhD students	73	99	95	207
Postdocs	130	106	63	239

Table 5.4: Number of doctoral students and postdocs (data from: April 2026). Persons who are present in more than one phase are counted in each phase that they are present.

KTT. As concrete success stories in academia, we can mention the examples of transitions to (assistant) professor positions of Julia Wiktor (Chalmers University of Technology, SE), Marco Gibertini (University of Modena and Reggio Emilia, IT), Giulia Palermo (UCLA, USA), Senja Barthel (Universiteit Amsterdam, NL), Antimo Marrazzo (SISSA, Trieste, IT), Anya Gryn'ova (University of Birmingham, UK), Kevin Jablonka (Technical University of Munich, DE), Michele Simoncelli (Columbia University, New York, USA), Rose Cersonsky (University of Wisconsin-Madison, USA), Rubén Laplaza Solanas (University of Sevilla, ES), Quansheng Wu (Institute of Physics, Chinese Academy of Sciences, CN), etc. Several of them will share an account of their research and their career path at the MARVEL final event at EPFL on 9 July 2026. We won't forget too the junior group leaders and software engineers at PSI, Empa, CSCS and EPFL, as part of the legacy of MARVEL there (Table 2.5).

As less successful measures, we can mention the original vision of a common doctoral programme and the later MARVEL Academy. These were strategically attractive but institutionally too difficult to implement in full. Semester structures and cross-university coordination limited what could realistically be formalized. The pandemic also interrupted activities and forced the postponement of some in-person schools. These were real setbacks, but MARVEL generally responded well: it pivoted to digital delivery, scaled recorded content, and then retained hybrid formats where they improved access.

5.3 Experiences and outlook

The implementation of MARVEL's education and training strategy reveals both unique advantages and logistical challenges. A major opportunity arose from the global shift toward remote learning during the pandemic. This catalyzed MARVEL's pivot toward digital education tools, allowing initiatives like the MARVEL Distinguished Lectures or the CECAM-MARVEL Classics in molecular and materials modeling to reach audiences of up to 600 unique attendees globally, vastly increasing the NCCR's reach. In addition, the recordings shared on Materials Cloud *Learn* and Lhumos platforms developed the visibility of such events. Since fall 2020, the number of unique visitors on the Materials Cloud *Learn* is quite stable, with an average of about 500 per month. Empowering junior researchers to take the lead in organizing seminars and retreats also proved highly rewarding, fostering at the same time effective internal communication of the research activities and the cultivation of soft skills and leadership among the young scientists.

Generally, MARVEL could benefit for collaboration with the home institution and its service units (SCITAS, Education Outreach Department). The longstanding partnership with CECAM (Centre Européen de Calcul Atomique et Moléculaire) was critical too. Externally, we can mention the Psi-k network or ICTP in Trieste. MARVEL now leaves behind a portfolio that can outlive the project: junior retreats and junior seminars as a tested community format; a summer camp for high school students that is being transferred to EPFL's Education Outreach Department with support of the Section of Materials (SMX); CECAM-MARVEL Classics in molecular and materials modeling, to share about the pioneering contributions in the field of molecular and materials simulations (e.g., major actors such as Roberto Car, Michele Parrinello, David Vanderbilt, Daan Frenkel, Lucia Reining, Shoshana Wodak or David Ceperley), and CECAM-MARVEL Mary Ann Mansigh Conversations, to gain a perspective on how modeling affects society (see Chapter 7); reusable open tools such as Quantum Mobile, OSSCAR and Lhumos, with infrastructural and network support from CECAM; MOOCs and recorded lecture series; and a set of international links through ASESMA, ASESMAnet, Psi-k, or ICTP. Ultimately, the final MARVEL-ICTP College in June 2026 is intended to draw PhD students and postdocs from multiple continents. The outlook is therefore not just to preserve successful formats, but to hand them over to stable institutional homes, letting them evolve over time to respond to the changing education needs of computational materials modeling, from the emergence of artificial intelligence to the integration of autonomous experiments and predictive materials design pipelines.

6 Equal opportunities

6.1 Strategies, aims and resources

MARVEL has been deeply committed to advancing equal opportunities within the computational materials science community, a field where women have historically been under-represented. Its core aims have consistently focused on a transversal strategy: raising gender awareness and ensuring an inclusive culture; enhancing the recruitment and career prospects of female scientists; preparing the next generation of women scientists by combating early stereotypes; and promoting work-life balance for all researchers.

Since the beginning, implementation relied on a close partnership with the Equal Opportunities Office and the Science Outreach Department at EPFL, with CHF 50’000 of funding allocated every year to the activities for children, particularly girls. The phase I portfolio established the core logic that remained visible throughout the NCCR: intervene across the whole pipeline, from school-age girls to early-career researchers, while ensuring that women were present as role models, mentors and leaders. The INSPIRE Potentials Master’s Fellowships started in 2016 (year 3) to attract excellent women Master’s students into computational materials science and convert part of this pool into future PhD candidates. With CHF 201’300 in phase I, CHF 457’000 in phase II, and CHF 350’734 in phase III, this is over 1 MCHF invested in the initiative over the entire program.

Phase II kept this architecture, but made it more measurable and more ambitious. Following the year 4 site visit and feedback from the SNSF Research Council, MARVEL strongly adapted its phase II strategy, moving from a mainly supportive strategy to a more structural intervention on climate, leadership and career progression, reallocating significant budget (roughly CHF 887’000 over years 5–8) to proactively and directly increase female presence in the NCCR. In particular, it formalized Agility Plus funding for junior women PIs, with a budget of CHF 420’000. In parallel, Clémence Corminboeuf joined the Executive Committee, which ensured that equal-opportunities considerations were also embedded at the level of strategic decisions.

Phase III consolidated this mature model, keeping women’s recruitment, visibility, and career progression as a central focus. A new Agility Plus effort with CHF 400’000 was created to give additional funding to women PIs. By this point, MARVEL had built a coherent portfolio spanning outreach, fellowships, leadership, climate, work-life balance, and institutional collaboration.

6.2 Highlights and overall impact

The strongest measurable achievement was at PhD level (Fig. 6.3). MARVEL set itself the explicit phase II goal of doubling the number of women PhD students, mainly through the MARVEL INSPIRE Potentials Master’s Fellowships, and it achieved this. Women represented 19% of MARVEL PhD students in year 3, 35% in year 7, stabilizing to a mean of 32% in phase III; in absolute terms the number of women PhD students more than doubled between year 3 (9 women PhD students) and year 7 (21 women PhD students, Fig. 6.3, top). The program proved transformative and this is the clearest sign that the equal-opportunities work had a concrete effect on scientific career entry in its own field.

The MARVEL INSPIRE Potentials Master’s Fellowships were the most successful instrument. It created an entry point into computational materials science for women students who might otherwise never have considered the field or a research career in it. In total, since its first call in 2016, 62 fellows were granted for a Master’s project in 24 different MARVEL groups in 8 institutions (Fig. 6.1). Of these, 19 have continued at the PhD level in a present or past MARVEL group. Of those who left, at least 24 have continued at the PhD level out-

Figure 6.1: *Current and previous INSPIRE Potentials fellows at the 2019 Review and Retreat at EPFL. From left to right: Jigyasa Nigam, Prof. Clémence Corminboeuf, Norma Rivano, Martina Danese, Julieta Trapé, Sinjini Bhattacharjee, Nataliya Lopanitsyna, and Dr Lidia Favre-Quattropani.*

Figure 6.2: *Summer camp for girls Matériaux super géniaux at EPFL, August 2025. Picture: EPFL Science Outreach Department.*

side MARVEL, in Switzerland or abroad. For those continuing at the PhD level in the field of MARVEL, the INSPIRE Potentials project was often crucial in the decision to stay in the domain. The fellowships therefore did more than raise visibility. They influenced concrete educational transitions and expanded the pool of young women entering a field where the pipeline is traditionally very narrow.

Another major accomplishment was the translation of equal-opportunities strategy into leadership opportunities. The phase II reorganization had temporarily reduced the share of women group leaders, but the Agility Plus scheme later brought four new women PIs into MARVEL, Sereina Riniker (ETH Zurich), Ana Akrap (UniFR), Emiliana Fabbri (PSI), Marta Gibert (UZH), and later, in phase III, Zoë Holmes (EPFL). As a result, the share of women among group leaders rose (Fig. 6.3, bottom). This matters strategically because it shows that targeted funding can correct structural imbalances more directly than awareness measures alone. It also increased the visibility of women researchers in project leadership, in decision-making, and in the scientific identity of the NCCR.

Looking at the share of women at different academic levels at EPFL for the different topics related to MARVEL (Fig. 6.4), we see a big difference between computer science and physics on the one side (share of women below 25% at all levels), and chemistry (share of women above 25%, even above 30% for PhD students) and, especially, materials science (above 30% at all levels), on the other side. Within MARVEL, the share of women at the postdoc and leader levels are comparable to the shares in physics (20%), those of PhD students being more in a higher tendency, as in chemistry or materials science.

A third strong area was the long-term work with girls and young women. In collaboration with the EPFL Science Outreach Department, MARVEL sponsored highly successful activities such as the *Polythème* workshop *Diamant, alu, caoutchouc, ils sont fous ces matériaux !*, the *Matériaux super géniaux* summer camp (Fig. 6.2), the chemistry and mathematics activities, and the *Coding club des filles*. Later, the MARVEL organized summer camp for high school students *Des atomes aux ordinateurs, à la découverte de la programmation scientifique* always set aside half of the spots for girls. This created a continuous presence from roughly age 7 to 19. These measures were repeatedly fully booked and renewed year after year, evidence of strong demand and credibility. Even if their direct long-term impact on later careers is hard to demonstrate within the funding period, their strategic value is high: they address stereotypes early, involve parents and schools, and create a future reservoir.

In terms of awareness and visibility, gender-bias trainings led by Prof. Marianne Schmid Mast (UniL) for both PIs and students were highly successful, fostering interactive and constructive discussions on overcoming implicit bias. A climate survey in 2020 described the work and gender climate as good, but many women and a substantial share of men still perceived career advancement as more difficult for women, and work-life balance remained gendered. The visibility of female role models was also championed through the #NCCRWomen campaigns and the Women in Materials artwork exhibition, which showcased female professors in EPFL's Institute of Materials, and now is extended to Chemistry, Physics and Mathematics Institutes at EPFL. MARVEL also ensured a good balance of speakers in the scientific events organized by

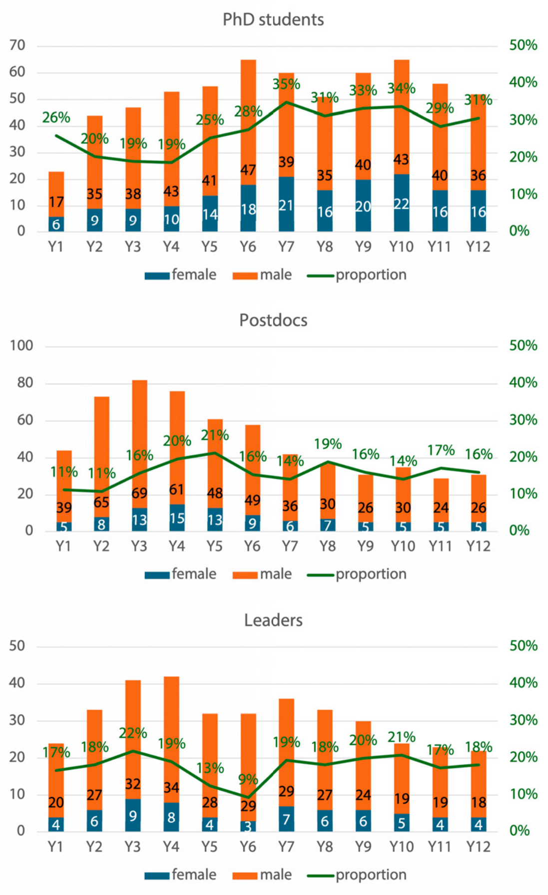

Figure 6.3: *Gender distribution of PhD students (top), of postdoc (middle), and of leaders (bottom) over the duration of the NCCR (data from April 2026). Left axes give the absolute numbers of women and men, right axes the share of women.*

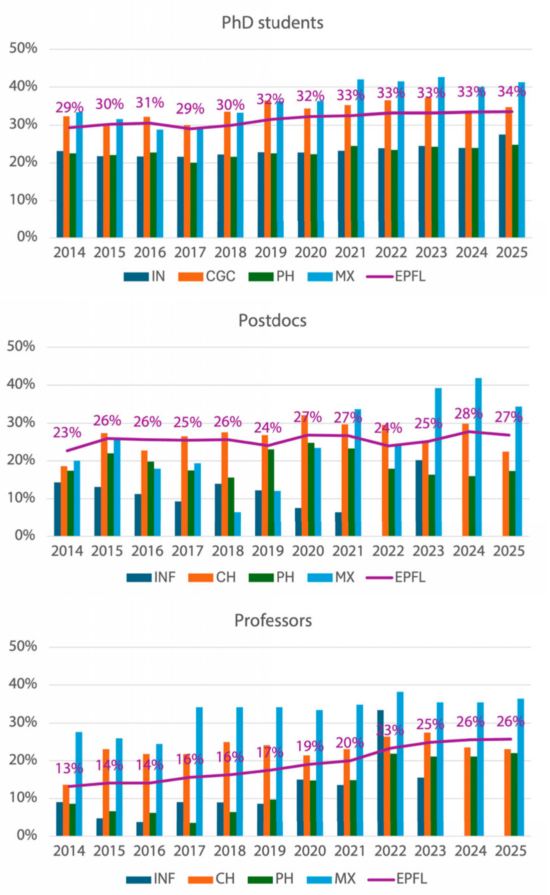

Figure 6.4: *Share of women at different academic positions at EPFL (top: PhD students, middle: postdocs, bottom: professors (all types)) in the fields of MARVEL (INF: computer science, CGC: chemistry, PH: physics, and MX: materials science) over the duration of the NCCR (source: EPFL Interactive gender monitoring).*

the NCCR (COMDI in 2018, Psi-k conferences in 2022 and 2025, internal events). The Junior Seminars started with 10% of women speakers in phase I, evolving to 26% in phase II and finally 41% in phase III, as a result of an active decision. 34% of all MARVEL Distinguished Lectures were delivered by women.

Some measures were less successful, or at least harder to scale. The recruitment of women into MARVEL-related fields remained constrained by the very small pool in physics, computer science, and parts of materials science. INSPIRE Potentials, despite its quality, often struggled to attract large applicant numbers because the field is narrow and many potential candidates were unfamiliar with doing a Master's project abroad. Participation in bias-awareness training also required repeated reminders, and not all PIs or laboratories were represented. This uneven engagement also highlighted a broader cultural challenge: many men in academia remain insufficiently aware of how long-established norms, informal power dynamics, and patterns of behavior associated with majority status can negatively affect women and other underrepresented groups in the field. Without greater recognition of these dynamics, efforts to improve inclusion often remain superficial. Finally, the attempt to create visiting fellowships for underrepresented PhD students and junior postdocs ran into legal and administrative funding constraints. These examples show that even strong measures do not automatically scale when structural, cultural, and regulatory barriers remain unchanged.

6.3 Experiences and outlook

Equal opportunities has always been central over the 12 years of MARVEL. The most effective measures were embedded in long-term and fruitful collaboration with the home institution and with service units that had operational expertise. EPFL's Equal Opportunities Office and Science Outreach Department were part of the delivery model and allowed the NCCR to leverage institutional expertise to run highly successful activities (summer camps and outreach for girls and children as well as for high-school students, training and mentoring for researchers, visibility actions and work-life-balance support). This collaboration deepened after the 2018 criticism, and the gender-bias awareness training developed for MARVEL with Prof. Schmid Mast also became a pilot for broader EPFL action on respectful behaviour and implicit bias (mandatory implicit bias training for faculty hiring committees).

Several key activities will remain as an institutional legacy. The INSPIRE Potentials Fellowships have now become a widespread concept in recent NCCRs. At EPFL, the MX Master fellowship program proposes a continuation to the MARVEL initiative, with the financial support mainly provided by the individual computational laboratories welcoming the students. The actions towards girls are fundamental of the activities of the EPFL Science Outreach Department and will continue after the end of MARVEL. Finally, the "Women in Materials" artwork, originally sponsored by MARVEL to highlight female leadership, will remain a permanent installation at EPFL, expanded now in the entrance halls of the Institutes of Physics, Chemistry, and Mathematics, ensuring lasting visibility for female role models and providing a daily inspiration for future generations of scientists

However, these efforts also highlighted important challenges. Cultural change cannot be achieved through isolated measures alone; it requires sustained leadership commitment, clear institutional accountability, and meaningful consequences when expected standards of inclusion and respectful conduct are not upheld.

7 Communication & outreach

7.1 Strategies, aims and resources

Across the full funding period, communication served a stable strategic objective: to make MARVEL's computational materials design and discovery paradigm visible, credible and usable, while building a collaborative community able to connect simulation, data, experiment and, ultimately, industrial uptake.

In phase I, the primary focus was on internal communication to build a committed community of researchers across different Swiss universities and facilities, foster synergies, align standards and workflows for data collection and exchange, and make collaboration routine through retreats, project meetings, distinguished lectures, the website and, later, junior seminars. External communication already existed, but it was largely supportive targeting scientific visibility, first contacts with industry, and broad public awareness centered around the idea that modeling and supercomputing could accelerate materials design and discovery.

In phase II, once the infrastructure had matured and platforms such as Materials Cloud and AiiDA were becoming visible, the strategy broadened from community-building to stakeholder-specific outreach, addressing industrial partners, external academic users, students, girls and young women, the public at large and policy makers. This phase professionalized the communication toolbox: internal, scientific and industrial newsletters were launched; feature stories and highlight papers became a regular editorial product; Twitter/X and LindedIn were added as relay channels; and press work was increasingly routed through EurekAlert. The LinkedIn private group was created with the intention of reinforcing ties within the MARVEL community and keep contacts with researchers. Even if probably underused, it helps to connect and follow MARVEL alumni.

In phase III, communication was explicitly tied to long-term legacy. Communication efforts were fine-tuned to maintain a strong public footprint while engaging policy makers, funding agencies, industrial partners, national laboratories, and supercomputing centers across Europe. Success stories, hybrid formats, alumni/community channels and the continued visibility of the Materials Cloud became key means of embedding MARVEL beyond the NCCR period. Resource allocation evolved to meet these shifting priorities. A fundamental change was the hiring of professional science communicators from phase II (Carey Sargent and then Nicola Nosengo).

Major adaptations over time were pragmatic and generally effective. Communication moved from an initially EPFL-centered structure to a more distributed network involving Empa, PSI, CSCS, CECAM and other partners. The pandemic forced a rapid transition to remote formats, but MARVEL turned this constraint into an opportunity by recording content systematically and later keeping hybrid formats for lectures, junior seminars and project meetings. In the concluding phase, the emphasis on curated success stories, interviews, and legacy channels (alumni group, recorded lectures, open platforms) shows a mature communication area that supports both accountability and long-term integration in the Swiss research landscape.

7.2 Highlights and overall impact

The most effective internal instruments were the ones that repeatedly brought the community together. The Review and Retreat became the backbone of internal communication: each edition gathered the majority of MARVEL members (about 130, Fig. 7.1), even the online 2020 edition, assisted alignment research goals and networking through poster sessions and junior highlight talks. The last four editions (2023 – 2026) took place in January in Grindelwald, with increasing success (Fig. 7.2). The MARVEL junior seminars, introduced in

Figure 7.1: The members of NCCR MARVEL at the 2017 Review and Retreat at EPFL.

2016 and later continued in hybrid mode, were also particularly successful. Organized by and for PhD students and postdocs, these seminars created a regular cross-group forum, opening on informal discussions around pizza, with an average participation of 40 to 60 people on site and 10-20 online.

Internal communication, onboarding, and shared identity were also supported by the dynamic MARVEL website and the regular internal newsletters. Externally, MARVEL built a diversified and increasingly professional portfolio. The website evolved from a project showcase into a continuous editorial channel with news, portraits, feature stories and science highlights (more than 170 up to now), which were shared through the scientific newsletters, appearing 9 – 10 times per year, with total of 78 in May 2026. The deployment of EurekAlert beginning in 2019 proved highly effective; press releases highlighting major scientific breakthroughs (61 issued over the last 6 years) regularly achieved thousands of views and were subsequently picked up by global science media platforms like Phys.org, SciTech-Daily, and Chemistry World. The launch of the @nccr_marvel Twitter/X account in 2017 was a resounding success, consistently boasting engagement rates between 2.5% and 4.27% — far above general higher-education benchmarks. The hits on the LinkedIn MARVEL page were equally substantial.

Several formats proved particularly successful because they translated a highly technical programme into memorable public experiences. The Ig Nobel Award Tour Show (Fig. 7.3) became a signature outreach event, drawing massive crowds (about 500 to 700 people) to celebrate “science that makes people laugh, and then think”, returning repeatedly, except during the pandemic. MARVEL strategically exploited different opportunities to showcase its research, taking advantage of large events at the host-institution (Scientastic and EPFL Open Days) or in other institutions (CSCS, PSI). Bespoke tools for sharing and explaining MARVEL output to the public were developed, including presence at interactive stands presenting 3D movies and hands-on experiments (e.g., explaining 2D materials, phonons, magnons, or sketch-map representation of materials’ landscapes) to engage thousands of visitors.

Figure 7.2: Poster session at the Grindelwald Review and Retreat in January 2026.

Figure 7.3: Ig Nobel Award Tour Show on 23 April 2026 at EPFL, with Marc Abrahams and the Bananas. Picture: Alain Herzog, EPFL.

Distinguished lectures were another very strong format. 41 were organized during the 12 years of MARVEL, 14 (34%) of them given by renowned female researchers. The switch to online delivery during the pandemic did not reduce impact and in fact expanded it, with an average of about 330 distinct connections for the 2020–2021 remote lectures and up to 670 for the most widely attended session. With the growing ties with CECAM, and after the invitation in 2017 of Mary Ann Mansigh Karlsen, an outstanding representative of the first generation of coders in molecular dynamics (Fig. 7.4), the CECAM-MARVEL Mary Ann Mansigh Conversations were launched to gain a perspective on how modeling affects society, addressing a broader range of topics and public than the distinguished lectures, with 50-70 attendees on site and up to 150 in total in hybrid format. In particular, we mention the ones on “Telling scientific stories — from science journalism to comics and visual storytelling” (with SWI swissinfo.ch sci-

Figure 7.4: *Mary Ann Mansigh Karlsen at EPFL on 15 November 2017, to share her recollection of the pioneering efforts of the first generation of coders. Picture: Alain Herzog, EPFL.*

ence and technology journalist Sara Ibrahim and director of the Istituto per le Applicazioni del Calcolo at the National Research Council of Italy Roberto Natalini), on "Science writing and science editing — from journals to journalism" (with *Nature Physics* editor Nina Meinzer and former *Nature/Chemistry World* news editor Mark Peplow), or the one with Erich Wimmer (Materials Design), addressing the fascination and industrial value of materials modeling. The CECAM-MARVEL Classics in molecular and materials modelling, already mentioned in chapter 5, were an equally successful and innovative hybrid format (with up to 500–600 attendees for some of them) that provided an opportunity, in particular for early career researchers, to interact informally with pioneers of the field of molecular and materials simulation, and benefit from their insights on technical matters and professional paths. Additional strengths were the visualization contests (in collaboration with the former EPFL ACCES (Application-Centered Computational Engineering Science) platform, the Julie Birenbaum art exhibitions, and later the success-story storytelling around emblematic achievements such as jacutingaite, topological materials, multiferroics, or the color of metals, as feature stories on the website.

The long term of the MARVEL project also offered the opportunities to experiment different formats, learn from the less successful, filter and refine efforts to maximize impact. For example, the CECAM/MARVEL movie nights were discontinued because attendance was too low, despite positive feedback from those who came, focusing instead on the highly successful Ig Nobel. Participating to initiatives from the host institution also provided valuable lessons. For example, a round-table on comics and science at the 2023 EPFL Open Days saw limited participation. On the other hand, a similar event at the science festival in Genova attracted a over 150 attendees. The Lunch@Lab event during the World Conference of Science Journalists produced engaged exchanges but drew fewer journalists than hoped. A lesson learned from these experiences is that appropriate communication is needed to highlight presence in large events with a rich and diversified program and a broad group of participants of different provenance and age.

7.3 Experiences and outlook

A central lesson from the funding period is that communication was most effective when it was closely coupled to real research outputs, visible platforms and existing institutional ecosystems. Collaboration with the host institution was important when appropriately tuned and offered seveal opportunities, e.g., collaboration with EPFL outreach structures for Open Days, Scientastic, and women-in-science activities, visualization contests and production of 3D movies for outreach activities with ACCES. Beyond EPFL, collaboration with CECAM, PSI, Empa, or CSCS broadened the reach of MARVEL and helped move communication from a single-site operation to a distributed network. The pandemic presented a major challenge by limiting face-to-face interactions, but it simultaneously unlocked the opportunity to embrace hybrid event models, which permanently enriched the accessibility of seminars and lectures for researchers residing in distant locations.

The most promising opportunities now lie in legacy and sustainability. MARVEL has learned that communication is not only dissemination but also infrastructure building: recorded distinguished lectures, CECAM-MARVEL Classics in molecular and materials modelling, and Mary Ann Mansigh conversations freely accessible on the Materials Cloud *Learn* and the new Lhumos platform, curated success stories, press-ready research highlights, newsletters, alumni channels, hybrid seminar formats, and public-facing demonstrations will remain useful after the NCCR itself ends. In strategic terms, these assets keep the scientific community engaged and make it easier for policy makers, funders, industrial partners, and service units to understand why MARVEL should outlive its original funding instrument. In particular, actions are being deployed to ensure that the MARVEL junior seminars, the Classics and Mary Ann Mansigh conversations will continue after the NCCR. The organization and management, of these events will be assured by engaged researchers (e.g., PhD students in groups currently in MARVEL and beyond, for the junior seminars) and build on the collaborative network consolidated by MARVEL, e.g., via the commitment of CECAM and its bespoke agreement with PSI and CSCS. The Lhumos portal will also continue to be developed and maintained with a specific MARVEL space via funding provided by CECAM and other partners. Finally, plans are being made to continue to hold retreat like events to preserve and expand collaborative actions in the Swiss materials research community. This resilient ecosystem will therefore ensure that the MARVEL legacy remains vital and fully integrated in the Swiss scientific landscape fulfilling the strategic goals of phase III.

8 Open science

8.1 Strategies, aims and resources

Open science is central to MARVEL and has been a foundational part of its core vision and backbone since the beginning. A key aim for the NCCR was to establish a self-sustaining long-term digital infrastructure for open simulations and data, extending the concept of FAIR (Findable, Accessible, Interoperable, and Reusable) data to encompass fully FAIR simulations.

In phase I, openness was primarily expressed through open-source software, provenance tracking and the first data-sharing infrastructure. AiiDA was released under an MIT license and the Materials Cloud began to emerge as the platform meant to connect raw data, curated data, workflows and educational content. The aim was to make computational materials research reproducible, shareable and reusable in practice.

During phase II, this initial infrastructure matured into a coherent open platform. The Materials Cloud became public and exposed the sections *Learn*, *Work*, *Discover*, *Explore* and *Archive*, while AiiDAlab and Quantum Mobile extended openness from code release to reproducible workflows and usable educational environments. The Materials Cloud *Archive* was then used as the open-data repository supporting the MARVEL data-management strategy, with already 19 MARVEL related entries in year 5 and about 60 in year 6 to almost 100 in the next 2 years. The strategic objective had clearly broadened from open codes to open workflows, open educational resources and FAIR data dissemination.

In phase III, Pillar 3 worked toward a self-sustaining digital infrastructure of open simulations and data. The Research Data Management (RDM) strategy gives the clearest statement of aims: *preserve all information needed to reproduce published results, publish datasets at the latest at the time of the publication of the related papers, use repositories that provide DOIs, versioning and long-term preservation, and progressively move from FAIR data toward FAIR simulations*.

The implementation of these policies was overseen by the scientific manager, who assumed the role of the overall data manager. The MARVEL Data Team, with one or two researchers per project, served as the relay for policy awareness, troubleshooting and training. The community was reminded of open-access requirements through newsletters, toolbox pages, Review-and-Retreat sessions and dedicated seminars. Resources were shared between the management team (data management, *Archive* moderation) and the Materials Cloud team inside the Open Digital Infrastructure (Pillar 3). MARVEL guaranteed at least 50’000 CHF/year for storage and sharing infrastructure, including 200 TB/year on CSCS `/store` and 10 TB/year of long-term storage prepaid for at least 10 years, while the broader digital-infrastructure (Pillar 3) budget of phase III amounted to CHF 1.3 million over four years. Furthermore, to support the increasing number of submissions and to enable long-term sustainability, MARVEL has transitioned its Materials Cloud *Archive* backend from a custom-built solution to the robust InvenioRDM framework (developed at CERN and the backbone of many large repositories including Zenodo).

8.2 Highlights and overall impact

Open science in MARVEL was not limited to a declaration in favor of openness, but was set by implementing and deploying robust open-science platforms and by establishing open-science-aware research practices throughout the MARVEL groups.

One strong achievement was to evolve Materials Cloud *Archive* from a MARVEL-built service into a repository for materials science data recommended by *Nature*’s *Scientific Data*, the European Commission’s *Open Research Europe*, and the Swiss National Science Foundation (SNSF). The *Archive* assigns DOIs, guaran-

	Phase I	Phase II	Phase III	All phases
Open access (gold, green, hybrid)	112 (31%)	525 (86%)	435 (97%)	1072 (75%)
Not open access	251 (69%)	82 (14%)	15 (3%)	348 (25%)
Total	363	607	450	1’420

Table 8.1: *Number and share of Open Access Publications (data from: April 2026).*

tees long-term preservation for 10+ years, and significantly boosts research visibility. Seven years after receiving its very first submission, it reached an important milestone on 3 April 2024 with the publication of the 1’000th record.

As outlined in Table 8.1 and in Fig. 8.2, the development of the open access publication share throughout the NCCR’s lifetime demonstrates outstanding progress. MARVEL evolved from a 31% open access rate in phase I to 86% in phase II, eventually achieving an exceptional 97% compliance rate in phase III. Some communities, such as chemistry, are historically more resistant to open science practices, with longer, non compliant embargoes and less fully open access journals, explaining the remaining 3% (1 to 6 articles per year, in phase III) non-open-access publications. The data side shows similarly strong progress, with most of the datasets underlying the research articles available open access at the time of publication (Fig. 8.2 and Table 3.2). We note that the lower number is explained by a fraction of publications being reviews or methodological/mathematical papers that do not necessarily come with datasets associated with them. On the other hand, we stress that several MARVEL papers involve the generation and publication of high-throughput datasets. These are extremely rich, and data is curated and annotated with relevant metadata. MARVEL is thus providing a large number of highly relevant, valuable, and impactful datasets. All of them are shared in the dataset index on the MARVEL website.

As highlighted in its report after the year-10 site visit, the review panel was *pleased by the world-leading activities in this area, where the consortium’s commitment has been strong since the beginning. Pillar 3 plans to establish a self-sustaining long-term digital infrastructure for open simulations and data, which of course directly feeds into this structure-related area. The panel was impressed by the way theMaterials Cloud Archive has evolved into a significant open science repository, extending its impact beyond MARVEL to benefit the wider scientific community, earning endorsements from the European Commission and the SNSF. Finally, the reviewers congratulate the person responsible for consistently educating and raising awareness among scientists regarding open access. The success of these efforts is obvious: almost all MARVEL publications adhere to SNSF policies, with a few exceptions due to embargoes.*

Beyond compliance and repository numbers, MARVEL also generated visible external recognition. In 2023, Nicola Marzari and collaborators won a special acknowledgment from the jury of the National Prize for Open Research Data (ORD) for their efforts in enabling data re-use (Fig. 8.3). The same year, MARVEL joined other NCCRs in a series of ORD meetings in Zurich, Lausanne and Basel, funded through the SNSF NCCR Network Ventures, making its open-science infrastructure part of a wider Swiss exchange on reproducibility and

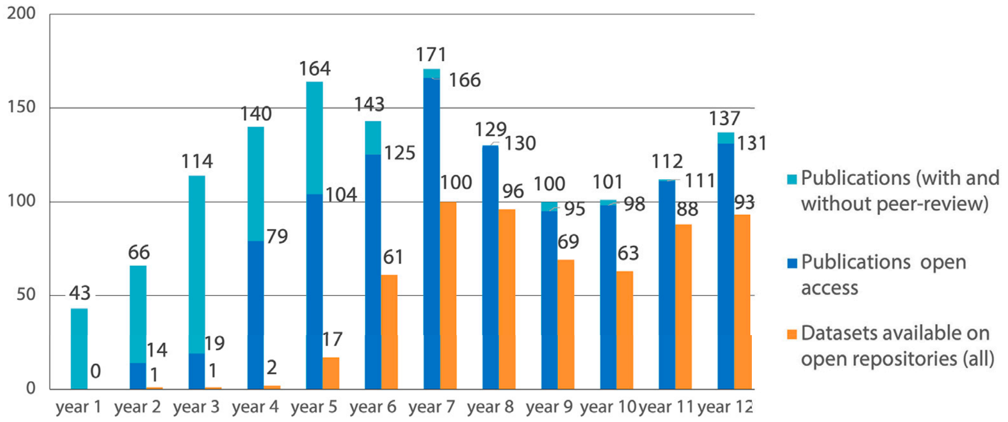

Figure 8.2: *Evolution of the number of publications, open access publications, and datasets during the time of MARVEL.*

Figure 8.3: Nicola Marzari (left), with Leopold Talirz and Giovanni Pizzi, former members of his lab and now respectively at Schott and PSI, with the special acknowledgment received on 6 December 2023 from the jury of the National Prize for Open Research Data, awarded by the Swiss Academies of Arts and Sciences.

data stewardship. The ETH Board's PREMISE project ("Open and reproducible materials science research"), with almost CHF 1.3 million of funding, further confirmed that MARVEL's open-data model had become a reference point beyond the NCCR itself.

8.3 Experiences and outlook

In the area of open science, CSCS has been an essential partner, providing robust storage infrastructures, Object Store capabilities, and a long-term storage service that forms the backbone of the Materials Cloud *Archive*. Institutional repositories at EPFL, PSI, Empa, ETH Zurich, and UZH have actively supported the green road to open access of publications.

As a legacy beyond the NCCR's funding period, MARVEL's open science infrastructure is designed to be self-sustaining. The Materials Cloud *Archive*'s data retention has already been prepaid to guarantee online preservation for at least 10 years after submission. The maintenance of moderation is planned to be absorbed by major external projects, including support by CECAM, while the continuation of the technical maintenance of the *Archive* is being discussed with HPC centers including CSCS and CINECA (Italy). MARVEL's numerous open-source code releases (e.g., QUANTUM ESPRESSO, CP2K, DFTK, Wannier90, Z2PACK, AiiDA, AiiDAlab, all listed on the MARVEL website) will persist as foundational simulation tools globally. Educational platforms like the Quantum Mobile virtual machine and the newly developed Lhumos learning platform will ensure that the educational legacy of MARVEL continues to train the next generation of computational materials scientists.

Crucially, both Empa and PSI now provide institutional deployments of AiiDAlab, demonstrating recognition of the platform's relevance. AiiDAlab's scope has expanded well beyond the original domain of computational materials science (as discussed in [87]), now encompassing fields ranging from quantum chemistry to atmospheric modeling. It has also been demonstrated to be effective in driving experiments in battery research and to support data analysis at large-scale facilities. Further support is evidenced by a two-year shared funding initiative at PSI (2026-2028) for a project scientist (E. Bainglass), jointly between Pizzi's group and the Center for Neutrons and Muons (CNM). The goal is to expand the adoption of AiiDAlab not only for simulations of neutrons and muons in matter — supporting and complementing experiments at PSI's large-scale facilities — but also as a platform for analysis of all data generated by neutron instruments at SINQ (PSI). Development of AiiDA and AiiDAlab remains open-source and continues to welcome external contributions, while maintenance will continue to be sustained within the groups of Pizzi (PSI) and Pignedoli (Empa).

The main challenge for long-term maintenance lies in the combination of increasing difficulty in securing funding for platform upkeep — since most research funding is directed toward activities whose impact is measured by the number of published papers, rather than the infrastructure that enables and supports them — and the academic context in which the work is embedded. In particular, long-term career paths for research software engineers remain insufficiently established, in contrast to the more standard trajectories of PhD students and postdoctoral researchers pursuing academic careers. As a result, even when funding is available, staff are often required to leave due to regulations limiting the maximum duration of employment for temporary academic positions. To partially address this issue, the two PIs, Pignedoli and Pizzi, have recently submitted a BRIDGE Discovery proposal to explore the integration of AiiDAlab developments with emerging AI technologies, with the aim of fostering industrial uptake and broader adoption of the platform, while also establishing an additional pathway for its long-term sustainability.

9 Feedback and concluding remarks of the NCCR director

This section looks back not at *what* MARVEL achieved, but at *how* the NCCR instrument shaped those achievements. The overall picture is positive: external review sharpened priorities, the SNSF framework pushed the consortium to think beyond publications, and the administrative layer, while demanding, made a complex national center governable. At the same time, the experience also shows that long-term research centers need room to adapt, stable support for people and infrastructure, and a realistic balance between ambition and administrative load.

9.1 NCCR assessment of review panel and SNSF

The review panel

Over the full funding period, the review panel appears to have played its most useful role when its feedback was concrete, timely and connected to decisions that MARVEL could actually implement. The annual meetings and site visits created regular moments of accountability. They forced the consortium to explain its choices clearly, not only to insiders, but to experienced outsiders who could judge whether the science, the structure and the use of public funds still matched the original mission.

The panel's recommendations had always direct practical effects. In the experimental validation platform, the criteria for the second call were revised after panel feedback so that proposals had to show a tighter link to MARVEL theory and a clearer balance between basic research and possible transfer potential. This was important because it pushed the experimental component to become more tightly connected to the center's computational core rather than growing into a parallel activity. In other words, the panel helped MARVEL become more integrated, not just larger.

A second visible impact came at the end of phase I. As a follow-up to the review panel's recommendations, MARVEL redirected recovered funding to launch a new set of collaborative projects, deliberately led by junior or newly arrived researchers and designed to build expertise for phase II. This was a smart response to external critique. Instead of treating evaluation as a formal hurdle, the leadership used it as a reason to refresh the portfolio, create new links across groups and prepare the next phase of the center.

The broader value of the panel was therefore not that it imposed a different scientific direction from outside. Rather, it provided disciplined pressure at the right moments. It helped the center sharpen selection criteria, think harder about collaboration, and avoid complacency. For a long-running center, that kind of pressure is healthy. It is especially helpful in a field like computational materials discovery, where methods change fast and where a promising direction can become outdated within a few years.

That said, the experience also suggests a limit. External review is most helpful when it judges direction, coherence and ambition, but does not over-prescribe. MARVEL benefited because it retained enough freedom to react to recommendations in its own way. The center could adjust selection criteria, launch new projects, and later reorganize from the original vertical-horizontal structure into grand challenges and finally into pillars. The lesson is that good review should be demanding, but should still leave room for scientific judgment inside the NCCR.

A posteriori, what would have been precious would have been also a more interactive engagement between the Director, a scientific leader from the review panel, and a NCCR program manager — if one could have had catch-up meetings every, say, 6 months it would have been possible and fruitful to brainstorm together on challenges and opportunities. For similar reasons, keeping the annual visits every year is very precious — the couple of times they were skipped it felt like a missed opportunity to engage and drive the project at some of its most critical juncture points.

The SNSF's Research Council

If the review panel was the main source of scientific challenge, the SNSF's Research Council had its strongest effect at the strategic level. The Research Council's influence can be read in the way MARVEL progressively widened its sense of responsibility. Over time, the NCCR was not assessed only as a collection of research projects. It also had to show progress in equal opportunities, education and training, knowledge and technology transfer, open science, communication, long-term integration and post-NCCR sustainability.

This broader framing was demanding, but in hindsight it was valuable. It prevented MARVEL from becoming only a successful grant for excellent scientists. Instead, it pushed the center to behave like a national public investment. This was visible, for example, in the equal opportunities agenda. The mini-site-visit with SNSF's Research Council members in 2019 signaled that these themes were not marginal. They were part of the core evaluation of the NCCR. The same applies to research data management, where MARVEL updated its strategy and submitted it to the SNSF for validation, and to crisis communication planning, which the center prepared in response to SNSF expectations in phase III.

The Research Council also mattered because it legitimized long-term thinking. One of the strongest features of the NCCR instrument is precisely that it allows Switzerland to support long-horizon projects that are internationally reviewed and expected to leave a structural legacy. MARVEL benefited from this logic. It could invest not only in papers and short projects, but also in infrastructures and institutions that require many years to mature, such as AiiDA, Materials Cloud and, later, the Laboratory for Materials Simulations at PSI.

Still, there is also a tension worth stating clearly. Strategic priorities introduced from above are rarely cost-free. In MARVEL's case, new center-wide efforts, including equal opportunities measures, required substantial internal reallocation of resources during phase II. Such reallocation was manageable because the center was strong, flexible and well led. But the lesson is that new expectations are easiest to absorb when they come with either extra resources or enough timing flexibility. Otherwise, the risk is that good strategic goals compete with already successful scientific activities for the same budget.

The SNSF's Administrative Offices

The role of the SNSF's Administrative Offices was less visible than that of the review panel or the Research Council, but no less important. Their contribution was not mainly intellectual or strategic. It was enabling. In a 12-year, multi-institutional program with changing personnel, evolving rules and several funding phases, someone has to make sure that contracts, reporting, compliance and formal procedures remain coherent. That work rarely appears in scientific highlights, but without it, a center like MARVEL becomes fragile very quickly.

The administrative interaction has been strongest in four areas. First, finance and reporting: the center repeatedly had to manage staff changes, institutional matching funds, reallocations between projects, and phase transitions. Second, governance: internal regulations were signed early and later updated. Third, compliance: open-access rules, data-management procedures and later crisis-communication planning all required formal follow-through. Fourth, continuity: validation steps and reporting routines created a shared rhythm across institutions that otherwise differ in internal practice.

The main positive point is therefore reliability. The Administrative Offices seem to have provided a framework within which a complex consortium could function predictably. The main negative point is equally clear: this predictability comes with a substantial administrative burden. For center leaders, this means time spent on documents, procedures and alignment, in addition to leading the science itself. That burden is not unique to MARVEL. It is a general feature of ambitious national instruments. The best conclusion is not that the administrative layer should disappear, but that it should remain proportional and as streamlined as possible.

9.2 Strengths, weaknesses of the NCCR instrument, challenges and lessons learned

The main strengths

The first and perhaps greatest strength of the NCCR instrument is time. Many important things that MARVEL achieved could not have been built in a three-year project. A national network across EPFL, ETH Zurich, PSI, Empa, CSCS, and several universities takes time. So does a culture of collaboration between theory, data, software and experiment. So do open digital infrastructures. Materials Cloud and AiiDA/AiiDAlab are good examples: they required repeated technical development, user uptake, governance, training, and community trust. A short project can produce a prototype. A NCCR can make it part of the research landscape.

The second strength is scope. The NCCR instrument can support not only research, but also structure. In MARVEL this was decisive. The center was able to combine frontier science with management, education, equal opportunities, communication, open science and knowledge and technology transfer. This made the center harder to run, but it also made the results more durable. MARVEL did not only publish. It changed how work was done, how data were shared, how young people were trained and how institutions collaborated.

The third strength is flexibility inside a stable framework. Over the years, MARVEL changed its scientific organization several times. It began with vertical and horizontal projects, then moved to grand challenges and incubators, and later to a pillar structure focused on legacy, open infrastructure, machine learning and long-term integration. The same center also launched Agility projects, experimental validation calls and phase-specific reallocations. This capacity to adapt is a major advantage of the instrument. It allows a center to react to scientific progress without being trapped by its original proposal.

A fourth strength is that the NCCR model gives national visibility and critical mass. It creates a common identity across groups that would otherwise collaborate more loosely. In MARVEL, this helped build links that almost certainly would not have emerged at the same scale without the center, especially between universities and institutions such as PSI, Empa and CSCS. This critical mass also mattered internationally, because it made Switzerland visible not only as a place with excellent individual groups, but as a coordinated ecosystem.

The main weaknesses and tensions

The strongest weakness of the instrument is complexity. A NCCR director and leadership team are not only scientists. They also become builders of institutions, coordinators of people, budget managers, public representatives and stewards of compliance. This is manageable when the management team is strong, but it is still a real cost. It reduces the time available for research and can create very uneven pressure on leaders. Critically, the extreme top-down nature of Swiss research institutions means that presidents/directors can stop any effort in its tracks, no matter how successful and/or visionary it is.

A second weakness is that phase-based funding can create cliff effects. In principle, phase transitions are useful because they force centers to justify continuation. In practice, they can destabilize successful activities. MARVEL experienced this in different ways: phase II budgets were front-loaded, which later forced reductions; one incubator was stopped early and another reduced; some platforms and projects were cut even while the overall program remained successful. This is not a failure of review. It is a structural tension in long-term programs that still need periodic re-approval.

A third weakness is that the instrument asks a center to succeed on many fronts at once. Scientific excellence remains the core task, but the center must also deliver on equal opportunities, education and training, communication, data management, knowledge and technology transfer, and structural legacy. These are all worthwhile goals. The difficulty is cumulative load. A NCCR needs enough management capacity and enough trust from its researchers for these added missions to strengthen the science rather than distract from it and MARVEL was always stretched thin on this.

Finally, sustainability remains a challenge built into the instrument. A NCCR can build a powerful infrastructure, but the infrastructure often outlives the funding cycle. This is especially true for software, repositories, data services and long-term training offers. The grant can create these assets, but host institutions and national partners should eventually carry them as they do — at massively larger costs and much reduced returns — for experimental facilities. This means the instrument works best when home institutions and partner institutions plan early for the post-NCCR phase.

Scientific and structural challenges, and the lessons learned

One important lesson from MARVEL is that broad scientific visions should be launched with room for later focus. The original design was useful for getting a national community started, but the center only reached full effectiveness after it reorganized around clearer problems and shared platforms. In that sense, the initial proposal did not fail. It did what early proposals often need to do: it opened a field and created a network. The more targeted formats of later phases then made the work more effective.

A second lesson is that platforms are as important as projects. Some of MARVEL's strongest legacies came from common infrastructure. The shared high performance computing (HPC) environment, the AiiDA workflow layer, data curation, Materials Cloud and common standards for reproducibility gave many projects a common language. This made collaboration easier and reduced duplication. It also helped the center survive personnel changes, because tools and workflows outlast individual appointments.

A third lesson is that theory-experiment links need active design. They do not happen automatically just because theorists and experimentalists are part of the same consortium. MARVEL's experience with PP7 is instructive. After early feedback, the center sharpened the criteria for experimental validation projects so that proposals had to connect more clearly to computational efforts and include real feedback loops. That was the right move. Where theory and experiment were tightly connected, the work gained both scientific strength and credibility.

A fourth lesson is that scientific roadmaps must be allowed to evolve. Some developments central to MARVEL's later identity were not equally central at the beginning. Machine learning became much more important over time. Open science moved from a useful principle to an operational backbone. Quantum computing emerged as a later opportunity. In phase I, metal-organic frameworks were added during the evolution of the center. These shifts were not signs of drift. They were signs that the NCCR remained alive to developments in the field.

A fifth lesson concerns people. Long-term centers are built not only by principal investigators, but by postdocs, PhD researchers, junior group leaders, program managers, data stewards and administrative staff. MARVEL repeatedly had to absorb departures, retirements, sabbaticals, career moves and even bereavement. The center managed this better because it could reallocate funding, bring in new researchers through Agility mechanisms, and rely on a stable management core. The lesson is simple: flexibility for people is not a secondary issue. It is part of research quality.

A sixth lesson came from external shocks. The COVID-19 period tested whether a distributed center could still function under disruption. MARVEL adapted by moving site visits, meetings and retreats online while keeping scientific and structural activity going. This resilience was helped by the fact that the center already worked digitally and had shared tools and routines. In that sense, infrastructure again proved to be a scientific asset, not just a technical one.

9.3 Conclusions and personal remarks by the NCCR director

Looking back, the strongest conclusion is that the NCCR instrument works best when it is allowed to do what only a long-term national center can do: build a community, build infrastructure and change habits. MARVEL did all three. It produced important science, but it also created a shared way of working across institutions and disciplines. That may prove to be its most lasting result.

From a director's perspective, one can also say that this instrument is demanding in the right way, but also over-demanding. It asks a center to think beyond the next paper. It asks whether the science is reproducible, whether young people are being trained, whether women and underrepresented groups are being supported, whether tools are being shared, whether institutions are being connected, and whether something useful will still stand after the grant ends. Those are not distractions from excellence. They are part of what excellence should mean in a publicly funded national program.

At the same time, the experience also encourages modesty. No NCCR can do everything equally well at every moment. Priorities have to be chosen. Budgets have to be shifted. Some promising directions have to be slowed so that more strategic ones can be protected. The most important leadership task is therefore not to preserve the original plan unchanged, but to preserve the center's purpose while allowing the implementation to evolve.

If there is one personal remark worth adding, it is this: MARVEL showed that a national research center can be more than a federation of strong groups. It can become a real shared project. When that happens, the value is larger than the sum of the grants. New collaborations become normal, digital tools become common goods, and institutions start planning together rather than in parallel. That is difficult to build, but once it exists, it changes the landscape.

A second personal remark concerns people whose names are often absent from summaries. Centers like MARVEL depend on researchers at every career stage, but they also depend on research software engineers, data curators, program managers, finance officers and communication staff. If Switzerland wants the legacy of such centers to last, it should not only preserve the science. It should also preserve the professional roles that make modern collaborative science possible. Open infrastructure does not run itself, and excellent coordination does not happen for free.

For that reason, one of the clearest lessons from this experience is that continuity after a NCCR should be planned not only as an institutional question, but also as a human one. The country needs career paths and stable support for the people who maintain shared software, curate data, support training and hold cross-institutional networks together. Without them, even strong scientific communities can slowly fragment once dedicated funding ends.

The final challenge is now continuity. The science will continue in many groups. The larger question is whether the habits, platforms and institutional links created by MARVEL will continue with the same clarity of purpose. The prospects are good, especially for the Materials Cloud and the Laboratory for Materials Simulations at PSI, but continuity will still require commitment from institutions and funders. The real success of the NCCR will be measured not only by what it achieved during its funding period, but by how much of that achievement remains active and useful afterwards.

Still, overall, notwithstanding all the major successes, this feels like a missed opportunity for Switzerland. The world of computational materials discovery has exploded, and startups in the field have received hundreds of millions of US$ in funding in the past year or two — from CuspAI (100 millions) to Lila Sciences (350 millions, now 550 millions), from Radical AI (55 millions) to Periodic Labs (300 millions). Google/Deepmind, Microsoft, Meta, to make a few, have published in the last couple of years major *Nature* papers on the field, and keep producing major and very visible efforts used worldwide. The Materials Project, that started not so much earlier than us, and was a pioneer in the field, has more than half a million users.

So, what I find surprising is that MARVEL had the very clear vision and the very supporting funding already in 2012 (preproposal) and 2014 (start date), but it was exceedingly difficult to push in unison such a pioneering effort.

A few items are worth mentioning, but ultimately I feel the responsibility for this missed opportunity, even if I do not know how I should have acted differently (being forceful (see below) was useless, and the requirement of building a community requires a soft touch ("herding cats", as one PI put it gently early on)). Interactions with the system were tough — universities and research laboratories in Switzerland are extremely pyramidal, and the leadership makes ultimately the vast majority of executive decisions, leaving very little operational capability. The in-depth bureaucratization enforced at EPFL in 2016–2024 has made anything faculty-driven very difficult to implement. And, last but not least, research groups are overfunded, with major income streams that do not depend on grants, making the community here less driven than what happens, say, in the US.

A few things really made life for MARVEL more difficult — these come from past administrations, so it's not particular helpful for the present or for the future, but it's food for thought in driving future efforts.

- The three tenure-track positions promised in phase I never really materialized, and turned out to be only a retagging of existing personnel (in some case outstanding MARVEL members). The real one promised for phase II was only approved at the very end of phase II, and became operational after all the plans for phase III had been already established.

- EPFL dismantled the possibility of having computational hardware that could be driven by faculty — this meant that all our database activities, user services, and agents couldn't be implemented in simple and reliable forms on site, but in complex and expensive on-the-cloud efforts that had to be periodically re-engineered. This drained our human and financial resources, and stopped core efforts in their track — I fought this to no end, but even as MARVEL director and president of the HPC commission at EPFL, there was a wall put forward by EPFL operations — and was a hard lesson on how top-down the system is.

- As mentioned earlier, the complexity of the AiiDA infrastructure put off almost all MARVEL PIs from engaging in high-throughput activities; also, it forced a choice between a student or postdoc learning science, or learning AiiDA.
- The abundant funding streams (either guaranteed, or with much fewer requirements than a NCCR) generate complacency — and the NCCR instrument requires so much involvement and effort that a community will not overly engage unless it's mission-critical to its survival — and this community was too successful (27 ERCs) to need the NCCR, or to ask itself in 2013–2014 what was the opportunity for Switzerland.
- On a personal note, although always keen on new challenges, I believe I would have not left EPFL if I could have had my research infrastructure here; that meant a few computer racks where to implement and deploy our capabilities. Instead, this was forcefully denied — actually the dean in 2016 acquiesced to the order of having our computer cluster removed and gifted. When a couple of years ago we donated our kitchen/common space to a new incoming assistant professor, and I saw major renovation work ongoing for more than one year to create some sparkling experimental laboratory for them (something for which I am delighted), while realizing that as NCCR director and full professor at EPFL I wasn't given any capabilities (as minor as a few computer racks) to perform my research, I understood it was time to move on.

Perhaps the most remarkable missed opportunity, for Switzerland, for Europe, and elsewhere, has been the failure to convince our leaders and policy makers that:

1. **our scientific society needs digital infrastructures and laboratories as much as it needs brick-and-mortar facilities;**
2. **digital rather than physical facilities can be shared worldwide in an open-source, open-access democratic model at no cost to arbitrary large communities;**
3. **the returns and impact of every franc, euro, or dollar, spent on sustained, long-term, digital efforts — as much as we need these latter, the allocations make no sense (CERN: 1'350–1'500 million euros of core budget in 2024; $\sim$ 1'000 papers.** QUANTUM ESPRESSO: **around 0.2 million euros in extramural funding; $\sim$ 5'000 papers).**

Every year we delay such basic and comparatively inexpensive action is a year lost to scientific progress.

In all of this, there remain extremely positive and powerful elements: the strategic efforts at PSI, CSCS, and Empa will remain, as is the strategic and community one with CECAM. The advances in electronic-structure and machine-learning efforts are world class. The Materials Cloud and AiiDA/AiiDAlab are very visible and some of the verification efforts (one for all, pseudopotentials) are extremely precious, foundational for the field, and would not have happened otherwise — remarkable that no one else in the world cared. Coding and agentic AI will greatly rely and benefit on what we have built and learned in these years.

Last and foremost, as I often repeat, materials enable the technologies that power our economies and sustain our society, and computational design and discovery of novel materials will remain firmly at the center of the research activities of the entire world for all our foreseeable future.

10

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Cover picture

Visualizing the quantum-to-chemical bridge: maximally localized Wannier functions transform complex electronic wave functions into intuitive, real-space orbitals. This mapping provides a powerful tool for understanding the chemical bonding and electronic structure of crystalline materials.
Illustration: Junfeng Qiao
Reference: Junfeng Qiao, Giovanni Pizzi, and Nicola Marzari, *Charting the electronic structure of experimentally known inorganic crystals*, under review (2026).

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