MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Materials' Revolution: Computational Design and Discovery of Novel Materials

Progress Report

Year 11

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Contents

1 Reaction to the recommendations of the review panel

We share here core passages from the report of the review panel, that was, broadly speaking, very positive on the current effort, and we highlight here the actions that we have taken in response to these comments.

General impression

The review panel continues to be very impressed by the content of the annual report and the presentations given during the review. In the ten years of the NCCR, the robust collaborative relationships among interdisciplinary research groups have facilitated the exchange of expertise, resources, and knowledge, resulting in significant breakthroughs in materials science research. Clearly, the enduring structural collaborations formed within MARVEL would not have been possible without this NCCR. Further, the consortium continues to be visible internationally. The panel noted that "international visibility" typically implies visibility in the USA and Europe. This is however not the case for NCCR MARVEL which has had a continual involvement with initiatives in Africa, such as ASESMA and ICTP-EAIFR, which the panel applauds. The panel does suggest that further regions such as South America and Asia could also be reached with educational workshops on AiiDA or Materials Cloud for example.

We thank the review panel for the kind words, and have taken, as always, at heart the suggestion to continue supporting a broad community of researchers worldwide. In fact, as part of our final series of events, we will have a 2-week school in the summer of 2026 organized together with the International Center of Theoretical Physics in Trieste (Italy), aiming to bring together students and young researchers from all regions, with full support for those coming from emerging economies. This will underline our efforts to support fundamental education in atomistic and quantum simulations, something for which the NCCR MARVEL has a long history in terms of workshops, schools, and online lectures. At the same time, the integration at PSI and Empa of data and simulation capabilities, through the Materials Cloud and AiiDAlab, continues our effort to provide "turnkey" solutions to the experimental community.
Online events in particular have been very successful — all recorded in *Learn* section of the Materials Cloud, and often offered in partnership with CECAM — and reaching tens of different countries beyond Europe and North America. The online format proved very useful during the Covid pandemic, and remains precious to address researchers in different geographical regions, and unburdened by travel constraints.

Scientific performance, collaborations and added value

Collaboration

The review panel has commended the consortium throughout the years for its high level of collaboration, which continues now that some senior members have left, and new PIs have been included, and about the added value of the NCCR scheme. Thinking about the final event in 2026, the experts will be interested to see a reflection on how the established collaborations are unique to a MARVEL approach, rather than natural continuations of the research of the individual PIs.

This will be done, and the final event at EPFL, as described later, will be also a moment of reflection, featuring a number of researchers that were active in different phases of MARVEL, and of young scientists whose career now span industry, academia, and startups.

The different projects also summarize their progress and performance below.

Pillar 1

There has been significant scientific progress since the last review on the metal alloys project, answering several of the scientific questions posed at that time. The research is certainly geared towards long-term scientific impact according to the reviewers and they are keen to see at the final event where this

research sits in the international state-of-the-art approaches using machine learning in this area.

Pillar 1 is focused on the design and synthesis of novel materials with an emphasis on metallic alloys, ceramics and technologically important materials. Machine-learning (ML) methods are being employed to explore the atomistic phenomena underlying phase transformations, deformation and diffusion mechanisms. This pillar's efforts in building ML models prioritize achieving sufficient accuracy for metallurgical applications, with researchers developing innovative approaches for challenging problems like solute-defect interactions and fracture models of multicomponent materials. This approach has enabled a systematic exploration of high-dimensional composition spaces to search for materials with optimal strength, ductility and durability. The recent addition of Christian Leinenbach from Empa has strengthened the pillar's research by facilitating closer integration between theory and experiment.

Regarding the metal-organic frameworks (MOFs) project, the panel is curious about the links of the computational workflow for assessing whether covalent organic frameworks (COFs) are suitable for photocatalysis to experiments. This project has the potential to elevate the research in a competitive area and ensure longer-term scientific impact. However, it is unclear to the experts whether this is a project of Professor Smit alone or whether other MARVEL PIs will continue working on it.

Thanks to a SNSF Advanced Grant to Professor Smit, the research in the field continues very strongly in Switzerland, maintaining strong connections between investigators and bridging theory with experiment.

Finally, the large-language models (LLMs) hackathon is praised by the reviewers, and if it is organized again, they will be interested in hearing more about the specific MARVEL contributions, its findings and its organization.

Professor Philippe Schwaller (EPFL) was invited to the Review and Retreat in Grindelwald in January 2025 to give a talk on "Teaching language models to speak chemistry: From design to synthesis".

Pillar 2

According to the review panel, the scientific added value, collaborations, and synergies have increased notably in phase III in this Pillar. The development of a modular software platform and methodological advances in machine learning and quantum chemistry have led to breakthroughs in materials design and discovery, as evidenced by high impact publications from the groups. Collaborations with partner laboratories, industry partners like BASF and Samsung, and external research laboratories further underscore the collaborative and interdisciplinary nature of the research efforts.
The reviewers also noted that the research is clearly geared towards long-term scientific impact, as evidenced by the focus on developing a high-quality software infrastructure, advancing the understanding of atomic-scale machine learning, and applying these methods to solve relevant materials science problems. The implementation of interactive apps on the Materials Cloud platform further demonstrates efforts to ensure visibility and usability, contributing to sustained progress for a transition to the post-NCCR phase.

We thank the review panel for these positive remarks and will continue on this line until the end of the project.

Pillar 3

The review panel agrees that Pillar 3 has increasingly become one of the success stories of the NCCR and plays a central role in MARVEL. The progress in all platforms including, but not limited to AiiDA and the Materials Cloud, have been exemplary. The panel in particular highlighted the new released versions of AiiDA along with the efforts to make it easier to use, the updates brought to Materials Cloud, as well as the releases of the Quantum Mobile virtual machine, where more properties can be calculated. The reviewers also stated that this Pillar has already had an international impact and will constitute one of the long-term impacts of the NCCR.
The panel further appreciated the candid discussion regarding uptake of AiiDA and criticism regarding its useability during the annual review. This is an issue encountered by many other software and the reviewers feel like the consortium is doing its best.

We thank the reviewers for acknowledging and praising the results of Pillar 3, and appreciating our current efforts on usability and uptake of AiiDA as a follow-up of the comments by the SAB/IAB. This is a clear area on which we have been focused in the past year and will continue to be a key focus area for the remaining 1.5 years of MARVEL.

Pillar 4

This Pillar dedicated to the legacy of the NCCR was already very convincing in year 9 and the review panel has only a few comments on it this year. The

development of M-stack in Pillar 2 and the development of many scientific infrastructures in Pillar 4 are overwhelmingly positive in the eyes of the experts, as they are at a phase where machine learning (ML) developments and integration of electronic structure methods and workflows is at a consolidation stage. The different developments and software packages are coming together through this Pillar and are being used by a rapidly increasing community in both academia and industry.
In addition, the new junior PIs are clearly bringing fresh air into the NCCR, as all of them have strong overlaps with MARVEL and several have been hired because of it. This suggests that a feedback mechanism has been established now in this research field in Switzerland, which is a very positive development according to the reviewers.

The activities at PSI and Empa, ignited by Pillar 4, are now fully established, and have lead to the creation of 4 positions at PSI (two group leaders, Pizzi and Schüler, and two scientists, Colonna and Timrov) and one at Empa (Yakutovich), creating the foundations for long-term structural efforts in the field.

ASM

The panel is pleased by the high quality of the results produced in this project. In particular, the collaboration between the different groups from the University of Fribourg, PSI, ETH Zürich and Empa would have been hardly possible without the NCCR. Further, methods such as "GW+DMFT" are currently used only in few groups worldwide and the activity within MARVEL is probably the most advanced one, which is also the case regarding the integration with a wider strategy for material characterization and design.
As commented last year, the connection with the main core of MARVEL activities is still relatively weak, although the reviewers noted that the efforts to improve in this direction are clear. For example, there is a connection with Pillar 3 towards automatization of the construction of pseudopotentials for photoelectron states and a natural link with Pillar 4 based on the development of integration between theoretical calculations of ARPES and other spectra with experimental activities at PSI.

We recognize that the link between the "Advanced Simulation Methods" project and the other pillars should be stronger. The last year and a half of MARVEL will be leveraged to strengthen the connection with other research groups. While keeping the existing links with Pillars 3 and 4 (automated creation of pseudopotentials and development of integration between theoretical calculations of ARPES and other spectra), we will start collaborating with Pillar 2 to introduce (more) machine learning acceleration techniques into our device simulations. Similarly, we will work with Pillar 1 to determine whether some of their newly discovered materials can be used as building blocks of future transistors, light-emitting diodes, or memristors.
As for the connection with industry, the programmed industry day was organized by Empa and EPFL and held at Empa in September 2024, with an attendance of around 100 scientists and high level talks from industry representatives, plus a keynote by Professor Roberto Car.

Bonus project, QS

According to the panel, progress since the last review has been substantial across various fronts: method development, interdisciplinary collaborations, generation of scientific added value, and alignment with long-term scientific impact goals. For example, the project has successfully developed and refined core methods aimed at bridging the gap between classical and quantum computing, and these methods have been extended from conceptualization to practical implementation, as evidenced by the development of novel approaches such as circuit knitting and adaptive schemes. Further, the project has fostered interdisciplinary collaborations within (with the groups of Philipp Werner and Nicola Marzari) and outside of NCCR MARVEL (with the efforts to interface classical electronic structure codes with quantum computing platforms, such as the interface between CP2K and Qiskit Nature, enabling the simulation of realistic systems). The review panel believes that the development of hybrid methods and novel algorithmic tools is particularly promising and goes beyond the capabilities of individual projects.
Overall, the research conducted in the bonus project is geared towards long-term scientific impact and has met most of the specific objectives outlined in year 9. The reviewers are looking forward to seeing the next steps towards integration with the rest of the NCCR and on applications which are more relevant for real-world problems.

While real-world applications remain a field-wide challenge in quantum computing, our focus on model Hamiltonians and fermionic systems provides a strategic pathway to understanding larger, practical problems. We are actively strengthening our collaboration with the NCCR's Pillar 2 on machine learning to identify opportunities where quantum computing and ML could synergistically address real-world challenges.

Structure-related areas

Education and training

The review panel congratulates the NCCR for continuing to provide activities in education and training of students and young scientists in all age groups. The reinstalment of the junior retreat post-COVID is very much appreciated and appears to have been a great success, fostering the young researchers' communication skills and expanding their professional networks. Initiatives such as summer schools and camps for high school students play a crucial role in inspiring the next generation of scientists. MARVEL's commitment to educational support is also evident to the reviewers through initiatives like the Open Software Services for Classroom and Research (OSSCAR) and The Learning Hub for Modelling and Simulation (Lhumos) platform.
Finally, the panel applauds the fact that the NCCR's efforts are not limited within Switzerland, but extend internationally with initiatives facilitating the exchange of African researchers among research groups within Africa and between Africa and Europe. These initiatives have proven instrumental in promoting collaborations and knowledge sharing, supporting the development of fundamental research in Africa. The reviewers suggest holding further educational workshops outside Europe too, possibly targeting Asia.

The College at ICTP as part as MARVEL final series of events, will gather largely PhD students and postdocs from all around the world, with a target of 30 students per continent, in addition to MARVEL students.

Knowledge and Technology Transfer (KTT)

As in previous years, the panel is impressed by the knowledge transfer activities of the NCCR. The continuous development and dissemination of Materials Cloud and of the AiiDAlab workflow frontend underscores the NCCR's mission to share their results with the wider and growing research community, making their tools and knowledge freely accessible. In addition, and as every year, MARVEL members have been involved in organizing conferences, tutorials or workshops, some sponsored by MARVEL.
Technology transfer has always primarily been restricted to the flow of trained personnel to industry rather than a transfer of research tools to industry. The reviewers believe that more could have been done regarding technology transfer, but at the same time, also appreciate that the NCCR has put tremendous efforts in all other aspects of the structure-related areas and that not all of them can reach the same level of achievement. The review panel is however pleased that the main topic of the junior retreat in 2023 was "Building bridges": between different research lines, but most of all between industry and academia. Further, the interviews of former MARVEL members who have joined the industry available on the website are very valuable as they share their experience and advice for younger researchers who are interested in careers beyond academia. Finally, the panel looks forward to hearing more about the industry day planned at Empa in the second half of 2024 in the final report.

An Industry day was organized at Empa on 5 September 2024. Some more details can be found in chapter 3, page 13.

Equal opportunities

The commitment of MARVEL to equal opportunities is exemplary in the eyes of the panel, who are particularly fond of the successful INSPIRE Potentials Master's Fellowships, the activities for girls and young women, the Agility Plus funding and the continued activities of the #NCCRWomen campaign.
The panel is pleased to hear that philanthropy channels are being explored to continue the INSPIRE potentials fellowships after the NCCR funding period. In addition, the reviewers strongly appreciate the thoughtfulness with which the anonymous feedback from INSPIRE potential fellows was dealt with and presented in this year's review.

The MARVEL community is convinced of the importance of a tool as the INSPIRE Potentials Master's fellowships. The costs are moderate (CHF 12'500 per student) for a high impact, and we are convinced that the groups would be willing to continue the activity by funding it on their own budget. In fact, the current plan is to move to a MARVEL legacy efforts, where the fellowships continue, but are self-funded by the individual investigators.
To make sure that everything goes smoothly during the research stay of the INSPIRE Potentials fellows and to avoid missing problems, we have added two actions: (i) in addition to a mentor in the group where they are staying, we propose an external mentor, if possible in the same institution but in a different group and ideally a former INSPIRE Potentials fellow, as a peer, to share any concern or just for support; (ii) we organize a small chat with the scientific manager after about 6 weeks, to check if everything is going well and to give them the opportunity to speak out, if needed.

Communication and outreach

The reviewers agree that the NCCR and its researchers are already highly visible internationally. This is of course guaranteed by the recognized excellence of the NCCR members and their published research but the versatile communication strategy, utilizing online platforms and in-person engagements clearly further enhances MARVEL scientists' visibility and disseminates research findings in an optimal way. The Psi-k conference in 2025 which will be again organized by the NCCR shall be another success according to the panel. Last but not least, the internal communication is facilitated by tools like newsletters, junior seminars, and successful retreats.

The Psi-k 2025 conference is currently being organized, and the full program is available on www.psik2025.net, with registration opening soon.

Open science

The review panel continues to be 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. As mentioned before, the panel is impressed by the way the Materials 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.*

We thank the panel for the very positive feedback and his continuous support on this topic.

Structural aspects and long-term plans

The reviewers believe that MARVEL has been successful beyond expectations in this aspect. Besides hiring new professors, including joint positions and interfaculty positions at EPFL, the NCCR has created sustainable digital infrastructures which will be beneficial in the long-term to the whole Swiss scientific ecosystem. The strengthening of the links with Empa, CSCS and PSI (and the creation of a new division there) has been a major achievement and the commitment of EPFL for financial resources to support hardware for Materials Cloud sustainability is also very positive. The legacy plans post-NCCR, focusing on strategic efforts in people, institutions, and infrastructure, were already in place at the end of year 9. The panel therefore has no further comments on this aspect and is convinced that the long-term impact and sustainable strengthening of the NCCR's research domain in Switzerland has been ensured.

Answers to the main recommendations of the review panel to the NCCR

To deliver an update on the "7 questions" in the final report.

This will be done.

To keep up the efforts with the industry regarding technology transfer in the remaining two years and to provide an update on the industry day planned at Empa in the second half of 2024 in the final report.

An Industry day was organized at Empa on 5 September 2024. Some more details can be found in chapter 3. As part of the final series of events of the NCCR, the event at EPFL will be in particular dedicated to the relevance of the scientific accomplishment of MARVEL to the industrial and technological ecosystem, inviting alumni that now lead research positions in industry and key players worldwide in industry.

To ensure that there is a good balance between female and male speakers at the final event, and to inquire, possibly by means of a survey, how female researchers and any other defined underrepresented group experienced the workload regarding equal opportunities over the course of the NCCR.

We will make sure to have a good balance between female and male speakers and teachers in the MARVEL final series of events, the Review and Retreat in Grindelwald, as this was the case, e.g., in January 2025, with 7 female speakers out of 26, the College at ICTP, and the event at EPFL.

To advertise training workshops for AiiDA even more widely, to reach researchers in Asia as well.

We are planning a new online AiiDA tutorial in 2025, similar to the past ones in 2020, 2021 and 2022, where we run twice the workshop (mornings and evening in Europe) to cover any timezone (for reference, past events/reports are available for 2020, 2021 and 2022).

2 NCCR Organisation

Dr. Christian Leinenbach is the head of the Advanced Processing & Additive Manufacturing of Metals group at Empa in Dübendorf. Since the beginning of phase III, he was associated to MARVEL Pillar 1, initially without funding. To reinforce Pillar 1 and experimental collaboration to validate the computational models for additive manufacturing with fabrication and testing of materials, it was decided to associate his group more formally to MARVEL, funding half the salary of a PhD student until the end of year 12. This was made possible through reallocation of funding. This also allowed to increase the MARVEL research funding of Anirudh Raju Natarajan (EPFL), also in Pillar 1.

As mentioned in last year report, Berend Smit (EPFL) left the project end of December 2023 and Bill Curtin (EPFL) retired at the end of April 2024, at the end of year 10.

The MARVEL management team is unchanged.

Thanks in part to support of MARVEL, Prof. Emmanouil Kioupakis (Univ. Michigan) is spending a sabbatical of one year at EPFL, initiating several collaboration projects with groups there.

As part of the effort of supporting junior female scientists, MARVEL provided a 6-month bridge funding for Dr. Maria Herz in the group of Prof. Fabian von Rohr at the University of Geneva. Dr. Maria Herz is working on the experimental synthesis of novel BCS superconductors predicted in the MARVEL team.

3 Highlights in research and structure-related areas from year 11

3.1 Highlights in research

You can find hereafter the list of highlights shared on our website, providing an in-depth picture of the research breakthroughs during year 11.

- In search of muons: Why they switch sites in antiferromagnetic oxides (groups of Giovanni Pizzi and Nicola Marzari)
- GPT-3 transforms chemical research (group of Berend Smit)
- Using machine learning to study the microscopic behavior of a solid-state electrolyte (group of Michele Ceriotti, Fig. 1)
- Computational study points to a promising Weyl semimetal (group of Nicola Marzari)
- Materials follow the 'Rule of Four', but scientists don't know why yet (group of Nicola Marzari)
- AiiDA used to drive experiments for the first time, matched with Empa's Aurora robotic platform (groups of Nicola Marzari and Giovanni Pizzi)
- In search of new alloys for aerospace applications (group of Anirudh Raju Natarajan, Fig. 2)
- A chain of copper and carbon atoms may be the thinnest metallic wire (group of Nicola Marzari)
- International collaboration lays the foundation for future AI for materials (groups of Sara Bonella, Nicola Marzari, and Giovanni Pizzi)
- A direct probe of the quantum geometry of materials (groups of Michael Schüler and Philipp Werner)
- A tool to explore the energy landscape of magnetic materials (group of Nicola Marzari)
- A paradigm shift in calculating the spectral properties of semiconductors (Nicola Colonna in the PSI group of Nicola Marzari)

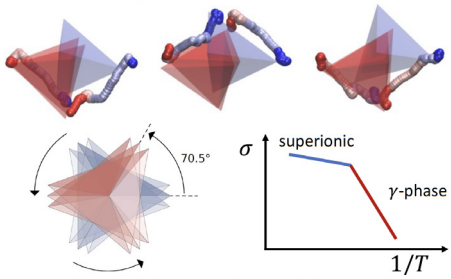

Figure 1: *Scientists in Michele Ceriotti's lab at EPFL have used machine learning to paint a more precise picture of how charge transport happens in lithium thiophosphate, a promising material for solid-state batteries.*

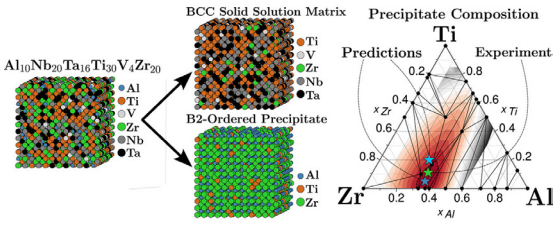

Figure 2: *A study by researchers in Raju Natarajan's group at EPFL has used computational methods to accurately describe the properties of a 6-component alloy made of aluminum, niobium, titanium, vanadium, zirconium and tantalum, which has promising properties that could be applied to aircraft engines.*

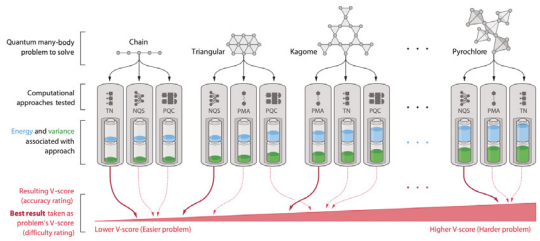

Figure 3: *A large collaboration led by MARVEL's Giuseppe Carleo has introduced a method to compare the performance of different algorithms, both classical and quantum ones, when simulating complex phenomena in condensed matter physics.*

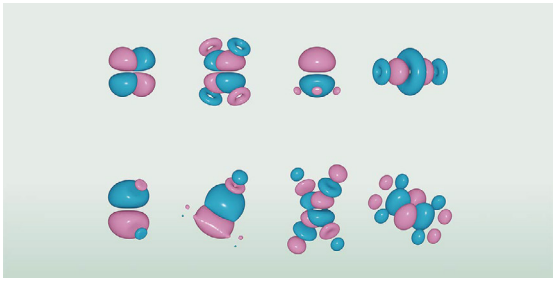

Figure 4: *Real-space depictions of maximally localized Wannier functions of a hafnium-diselinide monolayer, as described in a review article in* Reviews of Modern Physics *and highlighted on the journal cover, providing a map to the vast landscape of software codes that allow researchers to calculate Wannier functions, and to use them for materials properties predictions.*

- The best of both worlds: combining accurate spectroscopy and thermodynamics for correlated materials (group of Nicola Marzari)
- Computational marathon matches the efficiency of the AiiDA platform with the power of Switzerland Alps supercomputer (group of Giovanni Pizzi)
- A new benchmark to recognize the hardest problems in materials science (group of Giuseppe Carleo, Fig. 3)
- Orbitronics: new material property advances energy-efficient tech (group of Michael Schüler, cover picture)
- In search of the perfect materials for fusion reactors (group of Nicola Marzari)
- New widgets and extensions expand the OSSCAR platform for educational notebooks in materials science (groups of Sara Bonella and Giovanni Pizzi)
- How machine learning can help predict the spectral properties of materials (PSI group of Nicola Marzari)
- Mapping the ecosystem of Wannier Functions software (groups of Giovanni Pizzi and Nicola Marzari, Fig. 4)
- New machine learning approach enables accurate determination of Hubbard parameters at virtually no cost (group of Nicola Marzari)
- How to combine quantum and classical algorithms for materials simulation (groups of Jürg Hutter and Ivano Tavernelli)

3.2 Highlights in structure-related areas

In year 11, we have continued with all the previously engaged activities in Education and Training, Knowledge and Technology Transfer, Equal Opportunities and Communication. We will focus hereafter on the new activities and give a few updates.

Education and Training

We would like to highlight two new actions for Education and Training in year 11. The first one is the support of one scholarship for African students to attend a two-year Master's course at the ICTP-East African Institute for Fundamental Research (EAIFR) in Rwanda. The program is offered in three disciplines: condensed matter physics, physics of the solid-earth and high energy, cosmology and astroparticle physics. The first year is common to all fields. The second year is devoted to the specialized areas and culminates with a thesis. MARVEL-sponsored scholarship is aimed at students from African countries other than Rwanda, and preference has been proactively given to a female candidate.
The second action is the support of MARVEL to the new permanent exhibition "Materials in Motion" in the entryway of the EPFL campus's MXF building (Fig 5). It presents innovative engineering materials encased within resin blocks mounted on metal rods arranged around a central column, and accompanied by explanatory texts. The installation is the work of artists Etienne Krähenbühl and Alban Kakulya, and aims to present important engineering materials in an original and com-

Figure 5: *The new permanent exhibition "Materials in Motion" in the entryway of MXF building is the place to discuss new research projects.*

pelling way. The materials covered include crystals, perovskite solar cells, thermally drawn functional fibers, 3D-printed metals, dispersed microparticles, each with an explanation of the ongoing research surrounding it. MARVEL has contributed samples materials and contents on such topics as Weyl semimetals, solid-state batteries, and the "wonder material" Jacutingaite.

Other Education and Training activities included, as usual:

- the 6th MARVEL Junior Retreat in St. Moritz from 10 to 13 September 2024, gathering 60 participants; this year's theme was "entrepreneurship, technology transfer, intellectual property rights", and the goal was to help participants explore the opportunities for a career outside academia (Fig 6);
- 7 MARVEL Junior Seminars;
- 2 CECAM-MARVEL Classics in molecular and materials modelling, the first one on "Methods for computational biology and drug discovery" featuring Bill Jorgensen (Yale Univ.) and Shoshana Wodak (Flemish Free Univ. Brussels) on 5 June 2024 and the second one on "Quantum Monte Carlo methods in the continuum" with David Ceperley (Univ. Illinois Urbana-Champaign) on 27 January 2025;
- the Lhumos platform, as repository of domain specific training material in simulation and modeling, featuring interactive lectures, slide navigation, and comprehensive resources, has continued to be expanded, with new contents and in the view of gradually replacing the Materials Cloud *Learn* platform;
- the summer camp for high-school students "Des atomes aux ordinateurs" which took place from 24 to 28 June 2024; a new edition will take place from 23 to 27 June 2025, preparing at this occasion the transfer of its organization to the Education Outreach Department at EPFL;
- the participation to the EPFL information days for high-school students in November 2024, this year with an activity on Li-ion batteries, calculating the available voltage using data from the Materials Cloud three-dimensional crystals database (MC3D).

Figure 6: *A very attentive audience at the Junior Retreat in St. Moritz in September 2024.*

Knowledge and Technology Transfer

In this chapter, we would like to highlight the Industry day that took place at Empa on 5 September 2024, with an attendance of around 100 participants (Fig.7). The day-long workshop brought together members of industry, academia, and public research institutions to discuss areas in which computer simulations can provide important insights to industry.

Figure 7: *Question session after the keynote presentation by Prof. Roberto Car at the MARVEL Industry day at Empa on 5 September 2024.*

The workshop included invited seminars from academic and industrial partners. The keynote presentation for the event was given by Prof. Roberto Car from Princeton University. Speakers from companies such as IBM, BASF, Bosch, Microsoft, Schott and Beyond Gravity presented their outlook on how computer simulations can provide critical real-world insights to industry.

In year 11, we also continued to publish portraits of former members who have moved to industry after working as PhD students or postdocs in one of the MARVEL laboratories. Two new portraits were added to the four existing ones, Chiara Ricca, formerly in the group of Ulrich Aschauer and now with the chemical multinational company Dow, and Elsa Passaro, formerly with Nicola Marzari's group and currently senior software quality engineer at the open-source software company RedHat.
In addition, we can report on major advancements in AiiDA, Materials Cloud, AiiDAlab, Quantum Mobile, etc. and in EU projects, e.g., the 2024 Wannier Developers Meeting, with fifteen researchers meeting at the Paul Scherrer Institute for a hackaton and working on a new version of the Wannier90 code. MARVEL members organized or co-organized conferences, tutorials or workshops, with 19 in year 11, and some were also sponsored by MARVEL. All are listed in the NIRA database and on the website (nccr-marvel.ch/ctw). As example, we can mention the 12th edition of the International Conference of the African Materials Research Society (AMRS), held every two years since 2000, which took place in the Rwandan capital from 16 to 19 December 2024 (Fig. 8). MARVEL Director Nicola Marzari and CECAM Deputy Director Sara Bonella were featured among the speakers of the event, that gathered several hundred experts from around the world and focused on emerging themes in materials science, including biomaterials, energy materials, nanotechnology, sustainability, advanced materials and more.

Figure 8: *Panel on "Advancing gender equity in African research" that concluded the first day of the African Materials Research Society (AMRS) conference in Kigali in December 2024.*

Equal Opportunities

As a new topic in Equal Opportunities, we would like to mention the INSPIRE visiting PhD fellowships aiming at promoting international collaborations, while supporting young researchers from underrepresented groups (by gender, ethnicity, or any other status), with a special focus on women, and on researchers from sub-Saharan countries, in their career steps, developing their scientific network and increasing their self-confidence. They support PhD students and junior postdocs from outside the NCCR for a stay of 3 to 6 months in a MARVEL computational lab. The first recipient is Mitra Dowlatabadi (Fig. 9). As a PhD student at the University of Trieste, under the supervision of Antimo Marrazzo, she spent 3 months in the group of Nicola Marzari at EPFL for a fruitful collaboration, and will come back in 2025 for an additional 3 months. In a similar line, MARVEL provided a 6-month bridge funding for Dr. Maria Herz in the group of Prof. Fabian von Rohr at UniGE, supporting the experimental synthesis of novel BCS superconductors predicted in the MARVEL team.
During year 11, six new INSPIRE Potentials — MARVEL Master's fellowships were awarded to Katja Sophia Moos (in the group of Michael Schüler at UniFR), Maria Andolfatto (in the group of Nicola Marzari at EPFL), Cecilia Botta (in the group of Daniele Passerone at Empa), Niya Petkova (in the group of Giuseppe Carleo at EPFL), and Sofiia Chorna (in the group of Michele Ceriotti at EPFL), who received the fellowship twice, a first time for a 4-month summer internships and a second time for her 6-month Master's project (Fig. 9). We introduced this year the possibility to extend exceptionally the fellowships by 2 additional months, if this makes sense for the project and of course for the recipient. Also, to take into account some feedback received by recipients, to take care of their well-being, and to avoid missing problems, we have added two small actions: (i) in addition to a mentor in the group where they are staying, we propose an external mentor, if possible in the same institution but in a different group and ideally a former INSPIRE Potentials fellow, as a peer, to share any concern or just for support; (ii) we organize a small chat

Figure 9: *From left to right, the first INSPIRE visiting PhD fellow, Mitra Dowlatabadi, and the five 2024 INSPIRE Potentials fellows, Katja Sophia Moos, Maria Andolfatto, Niya Petkova, Sofiia Chorna, and Cecilia Botta.*

with the scientific manager after about 6 weeks, to check if everything is going well and to give them the opportunity to speak out, if needed. We also try to organize informal meetings for current and former recipients, as common coffee breaks on EPFL Campus or INSPIRE Potentials gathering at the Review and Retreat in Grindelwald. The current budget can cover three additional fellowships, which will be allocated after the next call, on 15 April 2025. This will be the last formal MARVEL call. The October 2025 call will take place and MARVEL management will take care of it. The funding will however come directly from the groups welcoming the selected students, as MARVEL legacy.

We took the opportunity of the presence of Shoshana Wodak for the CECAM-MARVEL Classics in molecular and materials modelling on "Methods for computational biology and drug discovery" to organize a lunch event for female students and postdocs at EPFL with her (Fig. 10), to give them the chance to discover her journey as a woman scientist and a pioneer of computational studies of proteins, and on career choices and decisions she took along the road. Shoshana's work, starting from the mid 1970s and continuing today, has contributed to shape the field with an inspiring combination of scientific and leadership skills. She has made seminal contributions in the study of protein interactions and has led advanced training programs, research teams, and promoted synergies between academic and applied research.

Figure 10: *Lunch event for female students and postdocs at EPFL with Shoshana Wodak on 4 June 2024.*

As already in the previous years, in 2024 MARVEL took part in 2 international events for women, (i) the International Day of Women and Girls in Science, with the invitation of CECAM on 14 February to discuss online with Shobhana Narasimhan (JNCASR, Jakkur, Bangalore and member of MARVEL's review panel) and MARVEL PhD student Virginie de Mestral (ETH Zurich) and share their experiences and perspective on women's access and participation in our domain; and (ii) the International Women's Day with MARVEL presence at the event "Sciences, feminine plural — How women can invest in science and technology" organized at EPFL on 29 February with the aim to highlight the careers of women in technical fields, to inform and discuss the role of EPFL and other players in advancing equality for women in these fields, and to network.

The project of artworks presenting female EPFL professors active in Physics, Chemistry and Mathematics in the entrance halls of the three institutes, similarly to the "Women in Materials" artwork in the Institute of Materials, is still ongoing. It is taking a bit more time than anticipated and should be visible by the summer 2025.

Of course, MARVEL continues to proactively make sure to have a good representation of women in all the activities it organizes or takes part to. Finally, MARVEL still supports the activities for young girls and boys, organized by EPFL Science Outreach Department, with always the same success.

Communication

During the last year, we have started planning and producing content to highlight some of the main "success stories" of NCCR MARVEL. In particular, one key goal of the project has always been to prove that theory, computations and experiments can work hand in

Figure 11: *The story of Jacutingaite at Scientastic at EPFL on 10 November 2024.*

hand, resulting in something that is more than the sum of each part. Some notable examples of these collaborations are shared on our website in the form of special features, with the first of the series revisiting how a close collaboration between theorists and experimentalists led to identify, synthesize and test a unique exotic material, Jacuntingaite, that until then had only appeared in some samples from a Brazilian mine. More are planned, as key communication action of MARVEL communication plan for the concluding phase (see Annex 3, page 24).

Building on this first success story, Lidia Favre-Quattropani, MARVEL scientific manager, told the story of Jacutingaite for a general public at Scientastic at EPFL in November 2024, a way for MARVEL to propose a different interaction with the public (Fig. 11).

Still for a broad public, MARVEL has been more recently involved in the exhibition "Shapes: Patterns in Art and Science" taking place at the EPFL Pavilion A from 17 January until 9 March 2025. The exhibition explores the richness of the natural and artificial patterns that surround us. Bringing together art, mathematics, materials science and biology, it highlights the shared fascination of scientists and artists with geometric, dynamic and symmetrical structures. MARVEL PI Michael Herbst is one of its curators and MARVEL could bring its support and network (Fig. 12).

Figure 12: *Michael Herbst presenting the materials science part of the exhibition "Shapes: Patterns in Art and Science" at its opening event on 16 January 2025 (Picture: EPFL — Alain Herzog).*

As other Communication actions in year 11, we had, as usually

- 4 Distinguished Lectures online or on hybrid format, with Dominika Zgid (Univ. Michigan) on "Ab-initio Green's functions methods for molecules and solids. What accuracy can we reach?", Massimiliano Di Ventra (UC San Diego) on "MemComputing: when memory becomes a computing tool", David Srolovitz (Univ. Hong Kong) on "Grain boundaries are natural Brownian ratchets: directional GB anisotropy", and Gerbrand Ceder (UC Berkeley) on "How the future of science may look: AI and autonomous laboratories for materials synthesis". An additional lecture with Alexandre Tkatchenko (Univ. Luxembourg) on "AI-Driven Fully Quantum Biomolecular Simulations" is planned in March 2025. The recordings of all are or will be available on the Materials Cloud *Learn* and Lhumos platforms.
- 1 CECAM-MARVEL Mary Ann Mansigh conversation on Science writing and science editing — from journals to journalism on 23 April 2024 with Nina Meinzer (Senior Editor at *Nature Physics*) and Mark Peplow (science journalist, regular contributor for *Nature*, or *Chemical & Engineering News*) to explore how scientific editing and scientific journalism work, how they are being transformed by new technologies, how young scientists can learn to better interact with editors and writers — or become editors and writers themselves (Fig. 13). Another one on "Science and Diplomacy" is planned on 28 February 2025, with the idea to address this topic from points of view that include ed-

Figure 13: *Mary Ann Mansigh conversation on Science writing and science editing on 23 April 2024 with Nina Meinzer.*

Figure 14: *Marc Abraham, the Ig Nobel Prize winners Chris Moulin, Minna Lyons, and Damien Bouffard, and the Bananas, gardians of time at Ig Nobel Award Tour Show on 16 April 2024 (Picture: EPFL — Alain Herzog).*

ucation and scientific exchange in developing countries, the potential of computational science as a facilitator for diplomacy, actions of international institutions promoting peace and disarmament, and the management of cooperative research infrastructures in problematic areas, with Gihan Kamel (SESAME, Jordan), Atish Dabholkar (ICTP, Italy), Tatsujiro Suzuki (RECNA, Japan), and Roland Bouffanais (UniGE, CH).

- After a 5-year break, on 16 April 2024, the Ig Nobel Award Tour Show came for the fifth time to EPFL (Fig. 14), with Marc Abrahams and the Ig Nobel Prize winners Chris Moulin, Damien Bouffard and Minna Lyons, giving a great evening talking about people who habitually stay up late, about sexual activity of anchovies, or about repeating a single word many, many, many, many, many, many, many times, and with the recording available online. A sixth edition will take place on 31 March 2025, with Marc Abrahams and the Ig Nobel Prize winners Mariska Kret, Marjolaine Willems, Roman Khonsari, Alexandra Sarafoglou, and Frantisek Bartos, and an evening about coin flipping, synchronization of heart rates of new romantic partners, or swirling of the hair of people in different hemispheres.

As internal events, we can mention the MARVEL Review and Retreat in Grindelwald on 13–15 January 2025 (Fig. 15), and before that, two series of hybrid projects meetings, one in June–July 2024 and one in October–November 2024 — each project meeting with all its members and open to other MARVEL interested members —, as well as the online (hybrid for MARVEL members) site visit in March 2024, gathering again the whole community. Finally we

Figure 15: *Group photo and poster session at the MARVEL Review and Retreat in Grindelwald in January 2025.*

can mention 9 internal and scientific newsletters, a continuous presence on the social media, namely on X and on LinkedIn, as well as continuing using Eurekalert to communicate research results to scientific journalists, publishing 8 press releases in year 11. Internally, a new channel on Slack has been set.

Open Science

We continue to inform and sensitize MARVEL scientists on open access requirements, for publications, for sharing the datasets underlying the publications, and for sharing their codes.
In year 11, all publications are available open access, in open access journals or on relevant repositories, except two publications under embargo. 98 datasets are available either on the Materials Cloud *Archive* or on another open repository. Seven years after receiving its very first submission, the Materials Cloud *Archive* has reached an important milestone on 3 April 2024 with the publication of the 1000th record.

4 Legacy of the NCCR and plans post-NCCR

As often highlighted, the legacy of the NCCR is built and ensured thanks to strategic efforts in three directions.

1. People: new PIs have been hired at EPFL and UniFR (Raju Natarajan, Herbst, Holmes, Schüler), group leaders and scientists at PSI (Pizzi, Timrov, Colonna) and Empa (Yakutovich), and software engineers at CSCS (Pintarelli) and EPFL, SCITAS (Fraux), together with close collaborations with CECAM (Bendinelli).

2. Institutions: the involvement of national laboratories and centers has been key and will be instrumental to sustainability post-2026.

3. Infrastructure: a core focus is and will be on the digital infrastructure for materials design and discovery — the codes, the workflows, and the Materials Cloud as the front-end dissemination platform.

Annex 1 Status of structural measures implementation

Planned measures according to annex 3 of the NCCR contract for phase III	Current status of implementation and comments
Infrastructure	
None	
Faculty	
Tenure-Track Assistant Professor in Computational Materials Science, phase II continuation (740 kCHF in-kind contribution, in addition to an expected 645 kCHF carry-over from phase II)	Prof. Anirudh Raju Natarajan was hired and started in February 2022
Additional measures	
None	

Specific conditions and requirements according to Article 10 of the NCCR contract for phase III	Current status of implementation and comments
None	

Annex 3 Planning of the NCCR conclusion and communication

A. Concept for the final event

After twelve years of the project and activities, the plan is to celebrate the end of MARVEL during the first semester of 2026, with a final series of events:

- a Review and Retreat in Grindelwald in January 2026,
- a 2-week College in computational materials science at ICTP in Trieste in June 2026, and
- a final event at EPFL in June–July 2026, including time for discussion with the review panel.

Review and Retreat in Grindelwald

We will have again the Review and Retreat in Grindelwald in January 2026. Everyone was extremely positive about the three editions we had there in 2023, 2024, and 2025 and it has always been a great community-building event. Since we also have Psi-k 2025 in Lausanne at the end of August 2025 (1'300 participants in 2022), instead of having the junior retreat in September 2025, we will have the junior researchers co-organize the January Grindelwald event, focusing squarely on the science and on their contributions, putting ahead the final achievements of MARVEL, rather than as a review (across the pillars and projects). For this last MARVEL Review and Retreat, MARVEL will support half of the costs for each participant. The rest of the costs will be paid directly by the groups.

College at ICTP in Trieste

We will organize a 2-week College (i.e., a 2-week school) in computational materials science at ICTP in Trieste. This will take place in June 2026, i.e., after college/university semesters end worldwide, so in the last 3 months (May–July) of MARVEL, in year 13. It will be directed by Nicola Marzari (MARVEL), Sara Bonella (MARVEL and CECAM), Michele Ceriotti (MARVEL), and Sandro Scandolo (ICTP), and is planning extensive lectures and exposure to our advanced simulations methods and tools. The College will gather about 240 PhD students and junior postdocs, including about 80 from the MARVEL community, and the worldwide community of peers in developed/developing countries, targeting roughly 30 students per continent, as a core educational event. The purpose is to disseminate our results with an open/democratic model: leverage our unique infrastructure to provide all the material right away and preserve it for long-term self-learning. We will have recorded lectures, self-learning tutorials, virtual machines containing all the tools and software; also, everything will be seamlessly and openly streamed worldwide.

The International Center for Theoretical Physics (ICTP) in Trieste, Italy, www.ictp.it, was created by Pakistani Nobel prize Abdus Salam in 1964. It conducts world-class research in frontier areas of science, and it is dedicated to fostering growth of advanced studies and research in physical and mathematical sciences through high-level scientific programmes, especially in support of excellence in the developing world to help bridge the knowledge divide. It is committed to science advocacy and international cooperation through science. Moreover, each year, ICTP brings together more than 6'000 world-leading and early career scientists from more than 150 countries to participate in advanced workshops and conferences that explore topics at the cutting edge of physics and mathematics. It is an UN organization governed by a tripartite IAEA/Italy/UNESCO agreement and has a memorandum of understanding with CECAM in place for joint initiatives, including access to HPC and leveraging its own international network (18 nodes in Europe, US, and Asia). ICTP will though contribute with its major and established scientific network worldwide,

and with a unique expertise in developing/emerging economies. Moreover we can count on

- its long-term integration in training environments,
- all organizational support (both for accommodation and travel),
- free accommodation for participants from developing countries, and for lecturers,
- very low cost accommodation (35 €/night per person in a double room) for all others,
- subsidized meals.

This event will energize a pool of outstanding early career and senior researchers in developed and developing scientific community (many often excluded from major initiatives), for maximal impact/democratization of MARVEL tools and output. It will allow the development/persistence of a world-class training program. It will provide a major leverage of MARVEL funding through ICTP contributions in organization/space/accommodation.

Final event at EPFL

We will organize a 1.5-day final event at EPFL, dedicated to the scientific accomplishment of MARVEL and to the relevance of these to the industrial and technological ecosystem, inviting alumni that now lead research positions in industry, alumnae from the INSPIRE Potentials fellowships, key players worldwide in academia and industry, representatives of partners institutions, such as ASESMAnet, Psi-k, CECAM, the SNSF review panel, MARVEL Scientific and Industrial Advisory Boards, EPFL leadership, and scientific journalists.
We will invite PIs of the first and second phases, such as Matthias Troyer (now at Microsoft Quantum in Seattle), Antoine Georges (now Director of the Center for Computational Quantum Physics, Flatiron Institute, Simons Foundation, in New York), Nicola Spaldin (ETH Zurich), Anatole von Lilienfeld (now at Univ. Toronto), Michele Parrinello (now at IIT, Genova), Bill Curtin (now at Brown Univ.), as well as members of our evaluating boards, such as Shobhana Narasimhan (JNCASR, Jakkur, Bangalore, review panel), Giulia Galli (Univ. Chicago, Scientific Advisory Board), and Boris Kozinsky (Harvard Univ., Scientific Advisory Board), to give their 12-year perspective on the MARVEL project.
The half-day before or after the event will be reserved for a meeting of the review panel, the MARVEL management, Executive Committee and leaders, and the representatives of EPFL to discuss and assess the final report. A dinner in a restaurant of the Lausanne area will also be organized for them.

B. Communication plan for the concluding phase

Research success stories

During year 12, the *Feature Stories* section of the MARVEL website will be populated with an ongoing collection of "Success stories" that will highlight some of the best examples of fruitful collaboration between theory, computation and experiments from all three phases of the project. The series was inaugurated in the fall of 2024 with an article on the story of Jacutingaite, an exotic material that was serendipitously discovered in 2008. MARVEL scientists eventually confirmed it as a rare example of a quantum spin Hall insulator (QSHI), and as the first ever material showing the so-called Kane-Mele physics.
A non-exhaustive list of other success stories to be published in the following months include:

- MARVEL's work on topological materials in phase II,
- MARVEL's theoretical/experimental collaboration on magnetoelectric multiferroics in phase I,
- Predicting the colors of metals from first principles,
- Type II Dirac Fermions, from prediction to experimental confirmation,
- The scientific legacy of Alexei Soulyanov (MARVEL member who passed away in 2019).

Portraits of researchers going to industry

We will continue the series of profiles of former MARVEL members who have moved into industry that started in 2023, aiming to add 6 more stories during year 12. The interviews, published on the MARVEL website in the *Technology Transfer* section, recount how the expertise and professional contacts developed as MARVEL PhD students and postdocs allowed many former members to develop a successful career in industries ranging from the chemical sectors to software houses, from automotive to electronics.

Artwork at EPFL

MARVEL has initiated and spearheaded the project of artworks showcasing female EPFL professors, starting with the "Women in Materials" artwork in the Institute of Materials. We have extended this to Physics, Chemistry and Mathematics, to be displayed in the entrance halls of the three institutes, with support from the School of Basic Sciences. Currently the last authorizations are being gathered (the buildings are listed) and the portraits should be installed by the summer 2025.

Video testimonials

Depending on available budget, we would like to produce over the course of year 12 short video interviews to summarize highlights from research projects, as well as to present direct testimonies of the positive impact of our activities in the fields of equal opportunity and education. The interviews (each 3 to 5 minutes long) will be professionally filmed and edited, with support from the in-house audiovisual services of EPFL and other participating institutions, and distributed through the NCCR MARVEL website and the Materials Cloud YouTube channel. A total of 12 videos would be produced, including interviews to the director, the leaders of the 6 main scientific pillars and projects, a selection of junior scientists and former INSPIRE Potentials fellows.

Website reorganization

Approaching the end of the project, the MARVEL website will be partially re-organized as a legacy resource that will no longer present updates on the projects' activities, but rather focus on showcasing the main results from the 12 years of the project and function as a gateway to the resources that MARVEL has developed for the scientific, industrial and educational communities. During the final months of MARVEL, we will maintain the same structure, but gradually shift focus away from news content and towards summaries of main achievements, completed with lists of publications, key stats, and other useful legacy information. At the end of the project, we will reorganize the home page by removing the lists of *Latest News* and *Upcoming Events* (links to the archived news and events will remain visible) and introducing summaries of the results of all main projects in phase III, as well as of the structural activities (Equal Opportunities, Education and Training, Knowledge and Technology Transfer).

Communication activities for the final series of events

Final event at EPFL

Science and technology journalists from Swiss media (e.g., *RTS*, *Le Temps*, *AGEFI*, *24 Heures*), as well as Italian, French and German ones will be invited to the final event at EPFL. Before it, we will prepare and circulate a press release about the event and conclusion of the project. We will coordinate with Mediacom (the EPFL communication unit) and be supported by them in inviting journalists to the event and distributing the press release more widely. An accompanying press kit will include an executive summary of the project's main achievements, fact-sheets on the results of individual projects, a selection of *Scientific Highlights* and *Success Stories* from the website, and a list of the main scientific publications from the three phases of MARVEL. The press kit will be made available online and printed copies will be distributed to the journalists participating in the event. The talks will be filmed and distributed online via YouTube after the event. Professional video and photography of the event will be produced in collaboration with Mediacom Events at EPFL.

College at ICTP

The talks will be live streamed and recorded for subsequent online dissemination, in collaboration with the ICTP Science Outreach department, to be presented on the Materials Cloud and our new LHUMOS platform (in collaboration with CECAM).

C. Financial implications

Budget for the review and retreat in Grindelwald

The budget of the Review and Retreat in Grindelwald is estimated to CHF 50'000, covering half of the cost for each participant. The rest of the costs will be paid directly by the groups.

Budget for the College at ICTP in Trieste

The MARVEL budget for the College at ICTP in Trieste is estimated to 189K€ and is presented in Table 3.1. MARVEL will cover the accommodation and food of its participants, as well as half the accommodation and food of participants from Europe and USA. For these two cat-

240 students	**Accommodation** 70 € for 2	**Travel**	**Food** 12 €/day
80 MARVEL	39K	(groups)	13K
80 Africa/Asia/Latin America	(ICTP)	80K	13K
80 US/Europe (covered for 50%)	20K	(groups)	7K
20 Lecturers (1 week each)	(ICTP)	15K	2K
Total: 189K	**59K**	**95K**	**35K**

Table 3.1: *MARVEL budget for the College at ICTP in Trieste, in €.*

egories, the travel will be covered directly by the groups of the participants. ICTP will cover all accommodation of all participants coming from developing countries, namely Africa, Asia, and Latin America, and MARVEL will cover their travel. 20 lecturers will teach one week each. Their travel and food will be covered by MARVEL and their accommodation by ICTP.

Budget for the final event at EPFL

For the final event at EPFL, we plan a budget of CHF 40'000, including

- travel and accommodation of invited speakers,
- travel and accommodation of invited participants,
- coffee breaks and standing lunches,
- a joint dinner with the review panel, the NCCR leaders and management, and EPFL representatives (covered by SNSF).

Budget for communication actions

For the communication actions, we plan a budget of 15'000, with

- CHF 2'000 for the website reorganization and hosting,
- CHF 6'000 for Nicola Nosengo's work for communication, May–July 2026,
- CHF 7'000 for video interviews.

Annex 4 Publications

All publications have been entered in NIRA, and are listed below with, when applicable, links to the datasets underlying the publications. We list publications either resulting directly from the NCCR (marked with a red hexagon ⬢) or with minor contributions from the NCCR. The publications marked with a green open circle (○) are accessible in Open Access (OA). The following lists cover the period February 2024 – January 2025.

1. Publications in journals with peer review, sorted by group leader
2. Publications in journals without peer review, sorted by group leader
3. Publications involving several groups or several projects (inter-group or inter-project)

1. Publications in journals with peer review, sorted by group leader

Phase III PIs

Group of Ana Akrap

⬢○ S. Nasrallah, D. Santos-Cottin, F. Le Mardelé, I. Mohelský, J. Wyzula, L. Akšamović, P. Sačer, J. W. H. Barrett, W. Galloway, K. Rigaux, F. Guo, M. Puppin, I. Živković, J. H. Dil, M. Novak, C. C. Homes, M. Orlita, N. Barišić, and A. Akrap

Magneto-optical response of the magnetic semiconductors $EuCd_2X_2$ ($X = P, As, Sb$)

Physical Review B **110**, L201201 (2024).

Group(s): Akrap / Project(s): AG+

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

○ I. Mohelsky, J. Wyzula, F. Le Mardelé, F. Abadizaman, O. Caha, A. Dubroka, X. D. Sun, C. W. Cho, B. A. Piot, M. F. Tanzim, I. Aguilera, G. Bauer, G. Springholz, and M. Orlita

Electronic band structure of Sb_2Te_3

Physical Review B **109**, 165205 (2024).

Group(s): Akrap / Project(s): AG+

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

Group of Sara Bonella

⬢○ D. Du, T. J. Baird, K. Eimre, S. Bonella, and G. Pizzi

Jupyter widgets and extensions for education and research in computational physics and chemistry

Computer Physics Communications **305**, 109353 (2024).

Group(s): Bonella, Pizzi / Project(s): P3

Links to article: Journal / Open access
Related datasets: doi.org/10.17632/7n2r2xh44k.1

⬢○ M. L. Evans, J. Bergsma, A. Merkys, C. W. Andersen, O. B. Andersson, D. Beltrán, E. Blokhin, T. M. Boland, R. Castañeda Balderas, K. Choudhary, A. Díaz Díaz, R. Domínguez García, H. Eckert, K. Eimre, M. E. Fuentes Montero, A. M. Krajewski, J. J. Mortensen, J. M. Nápoles Duarte, J. Pietryga, J. Qi, F. d. J. Trejo Carrillo, A. Vaitkus, J. Yu, A. Zettel, P. B. de Castro, J. Carlsson, T. F. T. Cerqueira, S. Divilov, H. Hajiyani, F. Hanke, K. Jose, C. Oses, J. Riebesell, J. Schmidt, D. Winston, C. Xie, X. Yang, S. Bonella, S. Botti, S. Curtarolo, C. Draxl, L. E. Fuentes Cobas, A. Hospital, Z.-K. Liu, M. A. L. Marques, N. Marzari, A. J. Morris, S. P. Ong,

M. Orozco, K. A. Persson, K. S. Thygesen, C. Wolverton, M. Scheidgen, C. Toher, G. J. Conduit, G. Pizzi, S. Gražulis, G.-M. Rignanese, and R. Armiento
Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange
Digital Discovery **3**, 1509 (2024).
Group(s): Bonella, Marzari, Pizzi / Project(s): P3, P4

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

Group of Giuseppe Carleo

D. Linteau, S. Barison, N. H. Lindner, and G. Carleo
Adaptive projected variational quantum dynamics
Physical Review Research **6**, 023130 (2024).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: github.com/dalin27/adaptive-pvqd

G. Gentinetta, F. Metz, and G. Carleo
Overhead-constrained circuit knitting for variational quantum dynamics
Quantum **8**, 1296 (2024).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.10829066

G. Gentinetta, A. Thomsen, D. Sutter, and S. Woerner
The complexity of quantum support vector machines
Quantum **8**, 1225 (2024).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.6303725

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

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 / Project(s): P2, QS

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

Group of Michele Ceriotti

S. Chong, F. Bigi, F. Grasselli, P. Loche, M. Kellner, and M. Ceriotti
Prediction rigidities for data-driven chemistry
Faraday Discussions **256**, 322 (2025).
Group(s): Ceriotti / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:6x-gs

W. B. How, S. Chong, F. Grasselli, K. K. Huguenin-Dumittan, and M. Ceriotti
Adaptive energy reference for machine-learning models of the electronic density of states
Physical Review Materials **9**, 013802 (2025).
Group(s): Ceriotti / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:s9-c5

F. Bigi, S. Chong, M. Ceriotti, and F. Grasselli
A prediction rigidity formalism for low-cost uncertainties in trained neural networks
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Related datasets: not applicable (review article)

Group of Daniele Passerone

M. L. Perrin, A. Jayaraj, B. Ghawri, K. Watanabe, T. Taniguchi, D. Passerone, M. Calame, and J. Zhang
Electric field tunable bandgap in twisted double trilayer graphene
npj 2D Materials and Applications **8**, 14 (2024).
Group(s): Passerone / Project(s): ASM

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:gq-6x

Group of Carlo Pignedoli

N. Bassi, X. Xu, F. Xiang, N. Krane, C. A. Pignedoli, A. Narita, R. Fasel, and P. Ruffieux
Preferential graphitic-nitrogen formation in pyridine-extended graphene nanoribbons

Communications Chemistry **7**, 274 (2024).
Group(s): Pignedoli / Project(s): P4

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:95-xw

G. Catarina, E. Turco, N. Krane, M. Bommert, A. Ortega-Guerrero, O. Gröning, P. Ruffieux, R. Fasel, and C. A. Pignedoli
Conformational Tuning of Magnetic Interactions in Coupled Nanographenes
Nano Letters **24**, 12536 (2024).
Group(s): Pignedoli / Project(s): P4

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:ze-41

M. Di Giovannantonio, Z. Qiu, C. A. Pignedoli, S. Asako, P. Ruffieux, K. Müllen, A. Narita, and R. Fasel
On-surface cyclization of vinyl groups on poly-para-phenylene involving an unusual pentagon to hexagon transformation
Nature Communications **15**, 1910 (2024).
Group(s): Pignedoli / Project(s): P4

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:6f-kw

X. Xu, A. Kinikar, M. Di Giovannantonio, C. A. Pignedoli, P. Ruffieux, K. Müllen, R. Fasel, and A. Narita
On-Surface Synthesis of Anthracene-Fused Zigzag Graphene Nanoribbons from 2,7-Dibromo-9,9′-bianthryl Reveals Unexpected Ring Rearrangements
Precision Chemistry **2**, 81 (2024).
Group(s): Pignedoli / Project(s): P4

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

C. Zhao, D. D. Bhagwandin, W. Xu, P. Ruffieux, S. I. Khan, C. A. Pignedoli, R. Fasel, and Y. Rubin
Dramatic Acceleration of the Hopf Cyclization on Gold(111): From Enediynes to Peri-Fused Diindenochrysene Graphene Nanoribbons
Journal of the American Chemical Society **146**, 2474 (2024).
Group(s): Pignedoli / Project(s): P4

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:62-ew

C. Zhao, Q. Huang, L. Valenta, K. Eimre, L. Yang, A. V. Yakutovich, W. Xu, J. Ma, X. Feng, M. Juríček, R. Fasel, P. Ruffieux, and C. A. Pignedoli
Tailoring Magnetism of Graphene Nanoflakes via Tip-Controlled Dehydrogenation
Physical Review Letters **132**, 046201 (2024).
Group(s): Pignedoli / Project(s): P4

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

A. Kinikar, X.-Y. Wang, M. Di Giovannantonio, J. I. Urgel, P. Liu, K. Eimre, C. A. Pignedoli, S. Stolz, M. Bommert, S. Mishra, Q. Sun, R. Widmer, Z. Qiu, A. Narita, K. Müllen, P. Ruffieux, and R. Fasel
Sterically Selective [3 + 3] Cycloaromatization in the On-Surface Synthesis of Nanographenes
ACS Nanoscience Au **4**, 128 (2024).
Group(s): Pignedoli / Project(s): P4

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:21-aj

N. Oinonen, A. V. Yakutovich, A. Gallardo, M. Ondráček, P. Hapala, and O. Krejčí
Advancing scanning probe microscopy simulations: A decade of development in probe-particle models
Computer Physics Communications **305**, 109341 (2024).
Group(s): Pignedoli / Project(s): P4

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.10563098

Group of Giovanni Pizzi

I. J. Onuorah, M. Bonacci, M. M. Isah, M. Mazzani, R. De Renzi, G. Pizzi, and P. Bonfà
Automated computational workflows for muon spin spectroscopy
Digital Discovery (2025), doi:10.1039/D4DD00314D.
Group(s): Pizzi / Project(s): P3, P4

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

D. Du, T. J. Baird, K. Eimre, S. Bonella, and G. Pizzi
Jupyter widgets and extensions for education and research in computational physics and chemistry
Computer Physics Communications **305**, 109353 (2024).
Group(s): Bonella, Pizzi / Project(s): P3

Links to article: Journal / Open access
Related datasets: doi.org/10.17632/7n2r2xh44k.1

M. Vogler, S. K. Steensen, F. F. Ramírez, L. Merker, J. Busk, J. M. Carlsson, L. H. Rieger, B. Zhang, F. Liot, G. Pizzi, F. Hanke, E. Flores, H. Hajiyani,

S. Fuchs, A. Sanin, M. Gaberšček, I. E. Castelli, S. Clark, T. Vegge, A. Bhowmik, and H. S. Stein
Autonomous Battery Optimization by Deploying Distributed Experiments and Simulations
Advanced Energy Materials **14**, 2403263 (2024).
Group(s): Pizzi / Project(s): P3
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:qt-1s

V. Blum, R. Asahi, J. Autschbach, C. Bannwarth, G. Bihlmayer, S. Blügel, L. A. Burns, T. D. Crawford, W. Dawson, W. A. de Jong, C. Draxl, C. Filippi, L. Genovese, P. Giannozzi, N. Govind, S. Hammes-Schiffer, J. R. Hammond, B. Hourahine, A. Jain, Y. Kanai, P. R. C. Kent, A. H. Larsen, S. Lehtola, X. Li, R. Lindh, S. Maeda, N. Makri, J. Moussa, T. Nakajima, J. A. Nash, M. J. T. Oliveira, P. D. Patel, G. Pizzi, G. Pourtois, B. P. Pritchard, E. Rabani, M. Reiher, L. Reining, X. Ren, M. Rossi, H. B. Schlegel, N. Seriani, L. V. Slipchenko, A. Thom, E. F. Valeev, B. Van Troeye, L. Visscher, V. Vlček, H.-J. Werner, D. B. Williams-Young, and T. Windus
Roadmap on methods and software for electronic structure based simulations in chemistry and materials
Electronic Structure **6**, 042501 (2024).
Group(s): Pizzi / Project(s): P3
Links to article: Journal / Open access
Related datasets: not applicable (review article)

M. L. Evans, J. Bergsma, A. Merkys, C. W. Andersen, O. B. Andersson, D. Beltrán, E. Blokhin, T. M. Boland, R. Castañeda Balderas, K. Choudhary, A. Díaz Díaz, R. Domínguez García, H. Eckert, K. Eimre, M. E. Fuentes Montero, A. M. Krajewski, J. J. Mortensen, J. M. Nápoles Duarte, J. Pietryga, J. Qi, F. d. J. Trejo Carrillo, A. Vaitkus, J. Yu, A. Zettel, P. B. de Castro, J. Carlsson, T. F. T. Cerqueira, S. Divilov, H. Hajiyani, F. Hanke, K. Jose, C. Oses, J. Riebesell, J. Schmidt, D. Winston, C. Xie, X. Yang, S. Bonella, S. Botti, S. Curtarolo, C. Draxl, L. E. Fuentes Cobas, A. Hospital, Z.-K. Liu, M. A. L. Marques, N. Marzari, A. J. Morris, S. P. Ong, M. Orozco, K. A. Persson, K. S. Thygesen, C. Wolverton, M. Scheidgen, C. Toher, G. J. Conduit, G. Pizzi, S. Gražulis, G.-M. Rignanese, and R. Armiento
Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange
Digital Discovery **3**, 1509 (2024).
Group(s): Bonella, Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: not applicable (no data)

P. Kraus, E. Bainglass, F. F. Ramirez, E. Svaluto-Ferro, L. Ercole, B. Kunz, S. P. Huber, N. Plainpan, N. Marzari, C. Battaglia, and G. Pizzi
A bridge between trust and control: computational workflows meet automated battery cycling
Journal of Materials Chemistry A **12**, 10773 (2024).
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:vx-ew

A. Marrazzo, S. Beck, E. R. Margine, N. Marzari, A. A. Mostofi, J. Qiao, I. Souza, S. S. Tsirkin, J. R. Yates, and G. Pizzi
Wannier-function software ecosystem for materials simulations
Reviews of Modern Physics **96**, 045008 (2024).
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: not applicable (review article)

M. Vogler, J. Busk, H. Hajiyani, P. B. Jørgensen, N. Safaei, I. E. Castelli, F. F. Ramirez, J. Carlsson, G. Pizzi, S. Clark, F. Hanke, A. Bhowmik, and H. S. Stein
Brokering between tenants for an international materials acceleration platform
Matter **6**, 2647 (2023).
Group(s): Pizzi / Project(s): P3
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:ph-jb

Group of Anirudh Raju Natarajan

Y. L. Müller and A. R. Natarajan
First-principles thermodynamics of precipitation in aluminum-containing refractory alloys
Acta Materialia **274**, 119995 (2024).
Group(s): Raju Natarajan / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:th-d5

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

S. Beaulieu, S. Dong, V. Christiansson, P. Werner, T. Pincelli, J. D. Ziegler, T. Taniguchi, K. Watanabe, A. Chernikov, M. Wolf, L. Rettig, R. Ernstorfer, and M. Schüler
Berry curvature signatures in chiroptical excitonic transitions
Science Advances **10**, eadk3897 (2024).
Group(s): Schüler, Werner / Project(s): ASM

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

Group of Berend Smit

J. Van Herck, M. V. Gil, K. M. Jablonka, A. Abrudan, A. S. Anker, M. Asgari, B. Blaiszik, A. Buffo, L. Choudhury, C. Corminboeuf, H. Daglar, A. M. Elahi, I. T. Foster, S. Garcia, M. Garvin, G. Godin, L. L. Good, J. Gu, N. Xiao Hu, X. Jin, T. Junkers, S. Keskin, T. P. J. Knowles, R. Laplaza, M. Lessona, S. Majumdar, H. Mashhadimoslem, R. D. Mcintosh, S. M. Moosavi, B. Mouriño, F. Nerli, C. Pevida, N. Poudineh, M. Rajabi-Kochi, K. L. Saar, F. Hooriabad Saboor, M. Sagharichiha, K. J. Schmidt, J. Shi, E. Simone, D. Svatunek, M. Taddei, I. Tetko, D. Tolnai, S. Vahdatifar, J. Whitmer, D. C. F. Wieland, R. Willumeit-Römer, A. Züttel, and B. Smit
Assessment of fine-tuned large language models for real-world chemistry and material science applications
Chemical Science **16**, 670 (2025).
Group(s): Corminboeuf, Smit / Project(s): P1, P2

Links to article: Journal / Open access
Related datasets: github.com/JorenBE/GPT-Challenge

M. J. Pougin, N. P. Domingues, F. P. Uran, A. Ortega-Guerrero, C. P. Ireland, J. Espín, W. L. Queen, and B. Smit
Adsorption in Pyrene-Based Metal-Organic Frameworks: The Role of Pore Structure and Topology
ACS Applied Materials & Interfaces **16**, 36586 (2024).
Group(s): Smit / Project(s): P1

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.10684869

Group of Ivano Tavernelli

L. E. Fischer, T. Dao, I. Tavernelli, and F. Tacchino
Dual-frame optimization for informationally complete quantum measurements
Physical Review A **109**, 062415 (2024).
Group(s): Tavernelli / Project(s): QS

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

S. Battaglia, M. Rossmannek, V. V. Rybkin, I. Tavernelli, and J. Hutter
A general framework for active space embedding methods with applications in quantum computing
npj Computational Materials **10**, 297 (2024).
Group(s): Hutter, Tavernelli / Project(s): QS

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:47-6g

A. Miessen, D. J. Egger, I. Tavernelli, and G. Mazzola
Benchmarking Digital Quantum Simulations Above Hundreds of Qubits Using Quantum Critical Dynamics
PRX Quantum **5**, 040320 (2024).
Group(s): Tavernelli / Project(s): QS

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

W. Dobrautz, I. O. Sokolov, K. Liao, P. L. Ríos, M. Rahm, A. Alavi, and I. Tavernelli
Toward Real Chemical Accuracy on Current Quantum Hardware Through the Transcorrelated Method
Journal of Chemical Theory and Computation **20**, 4146 (2024).
Group(s): Tavernelli / Project(s): QS

Links to article: Journal / Open access
Related datasets: github.com/dobrautz/tc-varqite-hamiltonians

Group of Vladyslav Turlo

M. Liyanage, V. Turlo, and W. A. Curtin

Machine learning potential for the Cu-W system

Physical Review Materials **8**, 113804 (2024).

Group(s): Curtin, Turlo / Project(s): P1

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:1m-0s

J. F. Troncoso, G. Lorenzin, C. Cancellieri, and V. Turlo

Explaining the effect of in-plane strain on thermal degradation kinetics of Cu/W nanomultilayers

Scripta Materalia **242**, 115902 (2024).

Group(s): Turlo / Project(s): P1

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:ah-f4

S. Gramatte, V. Turlo, and O. Politano

Do we really need machine learning interatomic potentials for modeling amorphous metal oxides? Case study on amorphous alumina by recycling an existing ab initio database

Modelling and Simulation in Materials Science and Engineering **32**, 045010 (2024).

Group(s): Turlo / Project(s): P1

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:ya-3k

G. Lorenzin, J. F. Troncoso, M. Liyanage, A. V. Druzhinin, L. P. H. Jeurgens, C. Cancellieri, and V. Turlo

Experimental and ab initio derivation of interface stress in nanomultilayered coatings: Application to immiscible Cu/W system with variable in-plane stress

Applied Surface Science **661**, 159994 (2024).

Group(s): Turlo / Project(s): P1

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:qx-7b

Y. Muller, A. Antušek, L. P. H. Jeurgens, and V. Turlo

Anomalously low vacancy formation energies and migration barriers at Cu/AlN interfaces from ab initio calculations

Scripta Materalia **248**, 116126 (2024).

Group(s): Turlo / Project(s): P1

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:kd-m4

G. Lorenzin, F. F. Klimashin, J. Yeom, Y. Hu, J. Michler, J. Janczak-Rusch, V. Turlo, and C. Cancellieri

Effect of residual stress and microstructure on mechanical properties of sputter-grown Cu/W nanomultilayers

APL Materials **12**, 101109 (2024).

Group(s): Turlo / Project(s): P1

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:nn-03

Group of Philipp Werner

S. Beaulieu, S. Dong, V. Christiansson, P. Werner, T. Pincelli, J. D. Ziegler, T. Taniguchi, K. Watanabe, A. Chernikov, M. Wolf, L. Rettig, R. Ernstorfer, and M. Schüler

Berry curvature signatures in chiroptical excitonic transitions

Science Advances **10**, eadk3897 (2024).

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

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:zq-tj

R. Mushkaev, F. Petocchi, V. Christiansson, and P. Werner

Internal consistency of multi-tier GW+EDMFT

npj Computational Materials **10**, 182 (2024).

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

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:9b-5n

V. Christiansson and P. Werner

Quaternary borocarbides: A testbed for DFT for superconductors

Physical Review B **109**, L180505 (2024).

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

Links to article: Journal / Open access

Related datasets: not applicable

J. Chen, F. Petocchi, V. Christiansson, and P. Werner

Nature of the photoinduced metallic state in monoclinic VO_2

Physical Review B **109**, L201101 (2024).

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

Links to article: Journal / Open access

Related datasets: zenodo.org/records/14599924

C. W. Nicholson, F. Petocchi, B. Salzmann, C. Witteveen, M. Rumo, G. Kremer, O. Ivashko, F. O. von Rohr, P. Werner, and C. Monney

Gap collapse and flat band induced by uniaxial strain in 1T-TaS_2

Physical Review B **109**, 035167 (2024).

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

Links to article: Journal / Open access

Related datasets: not applicable

Group of Lenka Zdeborová

L. Clarté, A. Vandenbroucque, G. Dalle, B. Loureiro, F. Krzakala, and L. Zdeborová
Analysis of Bootstrap and Subsampling in High-dimensional Regularized Regression
in *Proceedings of the Fortieth Conference on Uncertainty in Artificial Intelligence*, N. Kiyavash and J. M. Mooij, eds. (PMLR, 2024), vol. 244 of *Proceedings of Machine Learning Research*, pp. 787–819.
Group(s): Zdeborová / Project(s): P2
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:az-j9

G. Piccioli, E. Troiani, and L. Zdeborová
Gibbs sampling the posterior of neural networks
Journal of Physics A: Mathematical and Theoretical **57**, 125002 (2024).
Group(s): Zdeborová / Project(s): P2
Links to article: Journal / Open access
Related datasets: github.com/SPOC-group/numerics-gibbs-sampling-neural-nets

Phase II PIs, not active in phase III

Group of Ming Shi

S. A. Ekahana, Y. Soh, A. Tamai, D. Gosálbez-Martínez, M. Yao, A. Hunter, W. Fan, Y. Wang, J. Li, A. Kleibert, C. A. F. Vaz, J. Ma, H. Lee, Y. Xiong, O. V. Yazyev, F. Baumberger, M. Shi, and G. Aeppli
Anomalous electrons in a metallic kagome ferromagnet
Nature **627**, 67 (2024).
Group(s): Shi, Yazyev / Project(s): DD6
Links to article: Journal / Open access
Related datasets: not applicable

Group of Oleg Yazyev

R. Yadav, L. Xu, M. Pizzochero, J. van den Brink, M. I. Katsnelson, and O. V. Yazyev
Electronic excitations and spin interactions in chromium trihalides from embedded many-body wavefunctions
npj 2D Materials and Applications **8**, 56 (2024).
Group(s): Yazyev / Project(s): DD6
Links to article: Journal / Open access
Related datasets: not applicable

S. A. Ekahana, Y. Soh, A. Tamai, D. Gosálbez-Martínez, M. Yao, A. Hunter, W. Fan, Y. Wang, J. Li, A. Kleibert, C. A. F. Vaz, J. Ma, H. Lee, Y. Xiong, O. V. Yazyev, F. Baumberger, M. Shi, and G. Aeppli
Anomalous electrons in a metallic kagome ferromagnet
Nature **627**, 67 (2024).
Group(s): Shi, Yazyev / Project(s): DD6
Links to article: Journal / Open access
Related datasets: not applicable

2. Publications in journals without peer review, sorted by group leader

Group of Giuseppe Carleo

F. Metz, G. Pescia, and G. Carleo
Simulating continuous-space systems with quantum-classical wave functions
arXiv:2409.06415 (2024).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: github.com/frmetz/continuous-space-quantum-simulation

L. Mauron, Z. Denis, J. Nys, and G. Carleo
Predicting Topological Entanglement Entropy in a Rydberg analog simulator
arXiv:2406.19872 (2024).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.13318731

P. Tashev, S. Petrov, F. Metz, and M. Bukov
Reinforcement Learning to Disentangle Multiqubit Quantum States from Partial Observations
arXiv:2406.07884 (2024).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: github.com/mgbukov/RL_disentangle

Group of Clémence Corminboeuf

M. Haeberle, P. van Gerwen, R. Laplaza, K. R. Briling, J. Weinreich, F. Eisenbrand, and C. Corminboeuf
Integer linear programming for unsupervised training set selection in molecular machine learning
arXiv:2410.16122 (2024).
Group(s): Corminboeuf / Project(s): P2

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

Group of Michael Herbst

M. F. Herbst, V. H. Bakkestuen, and A. Laestadius
Kohn-Sham inversion with mathematical guarantees
arXiv:2409.04372 (2024).
Group(s): Herbst / Project(s): P3

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

Group of Zoë Holmes

S. Lerch, R. Puig, M. Rudolph, A. Angrisani, T. Jones, M. Cerezo, S. Thanasilp, and Z. Holmes
Efficient quantum-enhanced classical simulation for patches of quantum landscapes
arXiv:2411.19896 (2024).
Group(s): Holmes / Project(s): QS

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

A. Angrisani, A. Schmidhuber, M. S. Rudolph, M. Cerezo, Z. Holmes, and H.-Y. Huang
Classically estimating observables of noiseless quantum circuits
arXiv:2409.01706 (2024).
Group(s): Holmes / Project(s): QS

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

P. Bermejo, P. Braccia, M. S. Rudolph, Z. Holmes, L. Cincio, and M. Cerezo
Quantum Convolutional Neural Networks are (Effectively) Classically Simulable
arXiv:2408.12739 (2024).
Group(s): Holmes / Project(s): QS

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

Group of Nicola Marzari

L. Monacelli and N. Marzari
Electrostatic interactions in atomistic and machine-learned potentials for polar materials
arXiv:2412.01642 (2024).
Group(s): Marzari / Project(s): P2

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

C. Malica and N. Marzari
Teaching oxidation states to neural networks
arXiv:2412.01652 (2024).
Group(s): Marzari / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:w7-k1

Y. Shin, E. Di Lucente, N. Marzari, and L. Monacelli
The thermodynamics of $CaSiO_3$ in Earth's lower mantle
arXiv:2411.18489 (2024).

Group(s): Marzari / Project(s): P1

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

T. Carey, K. Synnatschke, G. Ghosh, L. Anzi, E. Caffrey, E. Coleman, C. Lin, A. Dawson, S. Liu, R. Wells, M. McCrystall, J. Plutnar, I. Plutnarova, J. Neilson, N. Marzari, L. D. Siebbeles, R. Sordan, Z. Sofer, and J. N. Coleman
A Portfolio of Electrochemically Exfoliated Two-Dimensional Materials: From Crystals and Simulations to Electronic Inks and Circuits
PREPRINT available at Research Square (2024), doi:10.21203/rs.3.rs-5319871/v1.
Group(s): Marzari / Project(s): P1

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

L. Binci, N. Marzari, and I. Timrov
Magnons from time-dependent density-functional perturbation theory and the noncollinear Hubbard formulation
arXiv:2409.19504 (2024).
Group(s): Marzari / Project(s): P4

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

S. Muy, T. Le Mercier, M. Dufour, M.-D. Braida, A. A. Emery, and N. Marzari
Optimizing ionic conductivity of lithium in Li_7PS_6 argyrodite via dopant engineering
arXiv:2407.15258 (2024).
Group(s): Marzari / Project(s): P4

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

B. K. Chang, I. Timrov, J. Park, J.-J. Zhou, N. Marzari, and M. Bernardi
First-Principles Electron-Phonon Interactions and Polarons in the Parent Cuprate La_2CuO_4
arXiv:2401.11322 (2024).
Group(s): Marzari / Project(s): P4

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

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Group(s): Marzari / Project(s): P4

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Group(s): Marzari / Project(s): P4

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Related datasets: not applicable

Group of Carlo Pignedoli

C. Zhao, L. Yang, J. C. G. Henriques, M. Ferri-Cortés, G. Catarina, C. A. Pignedoli, J. Ma, X. Feng, P. Ruffieux, J. Fernández-Rossier, and R. Fasel
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Group(s): Raju Natarajan / Project(s): P1

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

Group of Michael Schüler

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Related datasets: not applicable

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Group(s): Tavernelli / Project(s): QS

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Related datasets: not applicable

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Group(s): Tavernelli / Project(s): QS

Links to article: Journal / Open access

Related datasets: not applicable

T. A. Bespalova, K. Delić, G. Pupillo, F. Tacchino, and I. Tavernelli

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Group(s): Tavernelli / Project(s): QS

Links to article: Journal / Open access

Related datasets: not applicable

Group of Philipp Werner

Y. Murakami, D. Golež, M. Eckstein, and P. Werner

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arXiv:2310.05201 (2023).

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

Links to article: Journal / Open access

Related datasets: not applicable (review article)

Group of Lenka Zdeborová

L. Clarté and L. Zdeborová

Building Conformal Prediction Intervals with Approximate Message Passing

arXiv:2410.16493 (2024).

Group(s): Zdeborová / Project(s): P2

Links to article: Journal / Open access

Related datasets: not applicable

3. Publications involving several groups or several projects (inter-group or inter-project)

M. L. Evans, J. Bergsma, A. Merkys, C. W. Andersen, O. B. Andersson, D. Beltrán, E. Blokhin, T. M. Boland, R. Castañeda Balderas, K. Choudhary, A. Díaz Díaz, R. Domínguez García, H. Eckert, K. Eimre, M. E. Fuentes Montero, A. M. Krajewski, J. J. Mortensen, J. M. Nápoles Duarte, J. Pietryga, J. Qi, F. d. J. Trejo Carrillo, A. Vaitkus, J. Yu, A. Zettel, P. B. de Castro, J. Carlsson, T. F. T. Cerqueira, S. Divilov, H. Hajiyani, F. Hanke, K. Jose, C. Oses, J. Riebesell, J. Schmidt, D. Winston, C. Xie, X. Yang, S. Bonella, S. Botti, S. Curtarolo, C. Draxl, L. E. Fuentes Cobas, A. Hospital, Z.-K. Liu, M. A. L. Marques, N. Marzari, A. J. Morris, S. P. Ong, M. Orozco, K. A. Persson, K. S. Thygesen, C. Wolverton, M. Scheidgen, C. Toher, G. J. Conduit, G. Pizzi, S. Gražulis, G.-M. Rignanese, and R. Armiento

Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange

Digital Discovery **3**, 1509 (2024).

Group(s): Bonella, Marzari, Pizzi / Project(s): P3, P4

Links to article: Journal / Open access

Related datasets: not applicable (no data)

D. Du, T. J. Baird, K. Eimre, S. Bonella, and G. Pizzi

Jupyter widgets and extensions for education and research in computational physics and chemistry

Computer Physics Communications **305**, 109353 (2024).

Group(s): Bonella, Pizzi / Project(s): P3

Links to article: Journal / Open access

Related datasets: doi.org/10.17632/7n2r2xh44k.1

J. Van Herck, M. V. Gil, K. M. Jablonka, A. Abrudan, A. S. Anker, M. Asgari, B. Blaiszik, A. Buffo, L. Choudhury, C. Corminboeuf, H. Daglar, A. M. Elahi, I. T. Foster, S. Garcia, M. Garvin, G. Godin, L. L. Good, J. Gu, N. Xiao Hu, X. Jin, T. Junkers, S. Keskin, T. P. J. Knowles, R. Laplaza, M. Lessona, S. Majumdar, H. Mashhadimoslem, R. D. Mcintosh, S. M. Moosavi, B. Mouriño, F. Nerli, C. Pevida, N. Poudineh, M. Rajabi-Kochi, K. L. Saar, F. Hooriabad Saboor, M. Sagharichiha, K. J. Schmidt, J. Shi, E. Simone, D. Svatunek, M. Taddei, I. Tetko, D. Tolnai, S. Vahdatifar, J. Whitmer, D. C. F. Wieland, R. Willumeit-Römer, A. Züttel, and B. Smit

Assessment of fine-tuned large language models for real-world chemistry and material science applications

Chemical Science **16**, 670 (2025).

Group(s): Corminboeuf, Smit / Project(s): P1, P2

Links to article: Journal / Open access

Related datasets: github.com/JorenBE/GPT-Challenge

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 / Project(s): P2, QS

Links to article: Journal / Open access

Related datasets: doi.org/10.5281/zenodo.8263407

M. Liyanage, V. Turlo, and W. A. Curtin

Machine learning potential for the Cu-W system

Physical Review Materials **8**, 113804 (2024).

Group(s): Curtin, Turlo / Project(s): P1

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:1m-0s

S. Battaglia, M. Rossmannek, V. V. Rybkin, I. Tavernelli, and J. Hutter

A general framework for active space embedding methods with applications in quantum computing

npj Computational Materials **10**, 297 (2024).

Group(s): Hutter, Tavernelli / Project(s): QS

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:47-6g

P. Kraus, E. Bainglass, F. F. Ramirez, E. Svaluto-Ferro, L. Ercole, B. Kunz, S. P. Huber, N. Plainpan, N. Marzari, C. Battaglia, and G. Pizzi

A bridge between trust and control: computational workflows meet automated battery cycling

Journal of Materials Chemistry A **12**, 10773 (2024).

Group(s): Marzari, Pizzi / Project(s): P3, P4

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:vx-ew

A. Marrazzo, S. Beck, E. R. Margine, N. Marzari, A. A. Mostofi, J. Qiao, I. Souza, S. S. Tsirkin, J. R. Yates, and G. Pizzi

Wannier-function software ecosystem for materials simulations

Reviews of Modern Physics **96**, 045008 (2024).

Group(s): Marzari, Pizzi / Project(s): P3, P4

Links to article: Journal / Open access

Related datasets: not applicable (review article)

I. J. Onuorah, M. Bonacci, M. M. Isah, M. Mazzani, R. De Renzi, G. Pizzi, and P. Bonfà

Automated computational workflows for muon spin spectroscopy

Digital Discovery (2025), doi:10.1039/D4DD00314D.

Group(s): Pizzi / Project(s): P3, P4

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:yy-ds

S. Beaulieu, S. Dong, V. Christiansson, P. Werner, T. Pincelli, J. D. Ziegler, T. Taniguchi, K. Watanabe, A. Chernikov, M. Wolf, L. Rettig, R. Ernstorfer, and M. Schüler

Berry curvature signatures in chiroptical excitonic transitions

Science Advances **10**, eadk3897 (2024).

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

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:zq-tj

S. A. Ekahana, Y. Soh, A. Tamai, D. Gosálbez-Martínez, M. Yao, A. Hunter, W. Fan, Y. Wang, J. Li, A. Kleibert, C. A. F. Vaz, J. Ma, H. Lee, Y. Xiong, O. V. Yazyev, F. Baumberger, M. Shi, and G. Aeppli

Anomalous electrons in a metallic kagome ferromagnet

Nature **627**, 67 (2024).

Group(s): Shi, Yazyev / Project(s): DD6

Links to article: Journal / Open access

Related datasets: not applicable

Cover picture

Illustration of the hedgehog orbital-angular momentum texture in the chiral topological semimetal PtGa. The compound with opposite chirality exhibits opposite orbital angular momentum. Image credit: Monika Blentry, PSI (group of Michael Schüler, PSI and UniFR)
Reference: 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).

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