MARVEL

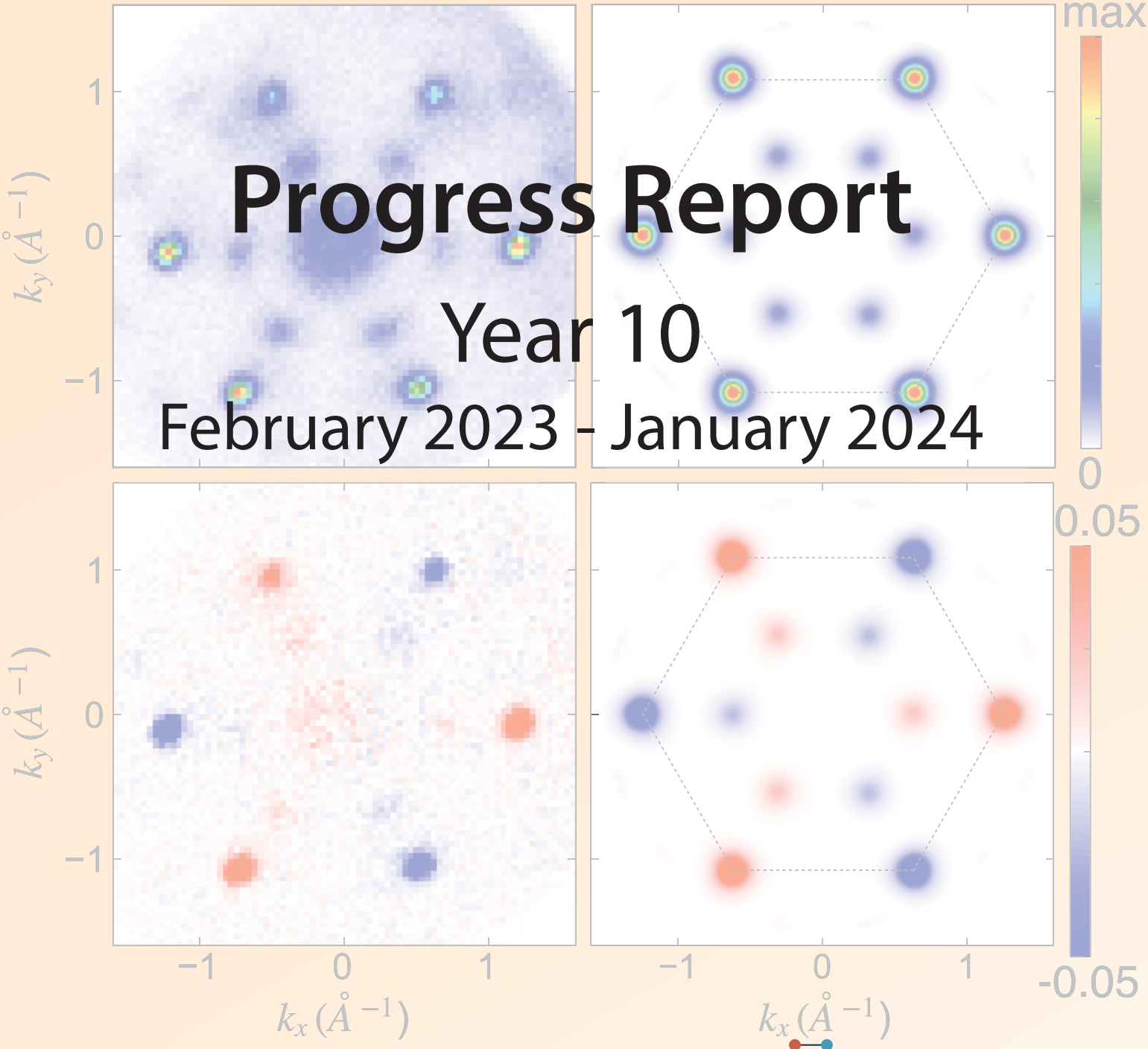
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Materials' Revolution: Computational Design and Discovery of Novel Materials

Progress Report

Year 10

February 2023 - January 2024



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Title of the NCCR	Materials' Revolution: Computational Design and Discovery of Novel Materials (MARVEL)
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Contents

1 Executive summary

The plans for MARVEL phase III are now fully developed and delivering — all the different Pillars and projects are ongoing, with regular project meetings and updates in between annual events (Review and Retreat, and Site Visit); closer collaborations have emerged also in the more recent efforts on Advanced Simulation Methods and Quantum Simulations ("Leveraging Quantum Computers and Algorithms for Materials Discovery"). Most notable in phase III has also been the arrival and engagement of new tenure-track faculty members (Anirudh Raju Natarajan in Materials at EPFL, on materials design and advanced manufacturing, Michael Herbst in Mathematics at EPFL, on the algorithms of electronic-structure calculations, Zoë Holmes in Physics at EPFL, on hybrid classical-quantum methods, and Michael Schüler in Physics at UniFR, on light-matter interactions), together with a closer involvement with CECAM thanks to the role and research of Sara Bonella. The creation of the new Laboratory for Materials Simulations at PSI (with 3 group leaders, 2 research scientists, and 20+ in personnel) is now complete, and is one of the core long-term structural deliverables from the NCCR, together with the creation of a Scientific IT division at Empa, and the long-term synergies with CSCS. EPFL has also reiterated its long-term commitment to the Materials Cloud, with additional CHF 150K in cash for years 11–12, to support long-term housing of the platform.

In order to focus the activities of the remaining full funding for MARVEL, the Director has established seven challenges for the PIs and the projects, to be answered in the remainder of the phase III:

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

We would like to focus both the March 2024 site visit, and the remaining time on MARVEL, on these 7 questions above — most are for the individual Pillars and projects, while the first and the last are broader.

In the meanwhile, we highlight below some of the key research and structural developments.

Pillar 1 Pillar 1 work has discovered new potential high-performance complex alloys using theory and advanced thermodynamics methods and has demonstrated the development and use of machine-learned interatomic potentials to discover new mechanisms of precipitation evolution and plasticity in lightweight metals. In addition, it has established screening protocols to assess whether a covalent-organic framework (COF) is a candidate for photocatalysis, and, notably, shown the applicability of large-language models in predictive chemistry.

Pillar 2 Pillar 2 has provided the first proof-of-concept of the M-stack framework, using the metatensor library to facilitate data exchange between ML descriptors and quantum mechanical calculators, supporting our effort to integrate atomistic machine learning and electronic-structure methods, including correlated wavefunction techniques. Collaborative efforts have further advanced our objectives towards reliable uncertainty quantification, and allowed us to demonstrate applica-

tions to NMR crystallography, alloy thermodynamics, and functional materials.

Pillar 3 Pillar 3 develops the digital infrastructure for exascale-ready accessible simulations, combining workflows (in AiiDA) with accelerated codes with robust algorithms (in SIRIUS). In year 10, AiiDA support has been strengthened for the Alps infrastructure, and scalability has been demonstrated on the GPU partition of LUMI, showcasing also SIRIUS improved robustness. Integration of the MaZe algorithms in SIRIUS is ongoing, and the team of Michael Herbst is now complementing Pillar 3, working on error control and novel robust algorithms. Together with Materials Cloud for FAIR data sharing, the Lhumos portal to share educational resources, and AiiDAlab for easy access to simulation capabilities, Pillar 3 works toward the delivery of a self-sustaining long-term digital infrastructure of open simulations and data.

Pillar 4 The integration of MARVEL in the Swiss scientific landscape is also now established, with the fully staffed Laboratory of Materials Simulations at PSI (20+ scientists and students) moving to new headquarters in September 2023. Core activities are driven by the three groups on "Materials Software and Data", "Multiscale Materials Modelling", and "Light-matter Interactions", and two tenure-track scientists on electronic-structure methods. These activities are matched by complementary efforts at Empa, where a new Scientific IT division has been created, and the engagement of CSCS where the new PSI HPC resources will be deployed on the Alps architecture of GraceHopper virtual cluster. The research focus remains firmly in the support of the experimental capabilities, with a focus on computational spectroscopies.

Advanced Simulation Methods Methods and tools based on Green's functions are developed in the project to simulate complex materials and realistic devices. At the device level, progress has been made on the treatment of electron-phonon interactions and impact ionization. On the materials side, the development of a user friendly multi-tier GW+DMFT framework is under way.

Quantum Simulations The Quantum Simulations project is working on hybrid quantum algorithms to combine classical and quantum computing for electronic structure calculations. This year the focus was on simulating dynamics of quantum systems with diverse hybrid approaches, as well as on the application of quantum machine learning for the simulation of continuous space systems and material characterization.

Structure-related aspects Like in previous years, we participated in — and organized directly — several meetings and events that contributed to straighten the position of MARVEL in the Swiss community and at the international level, while also disseminating the results of our research. These included the PASC23 Conference in Davos, the CECAM-Psi-k Conference in Berlin, as well as key educational events such as the Advanced QUANTUM ESPRESSO school in Pavia or the Machine Learning Interatomic Potential School for Young & Early Career Researchers (MLIP 2023). All are listed on the website (nccr-marvel.ch/ctw).

Our portfolio of open-source resources for the community has grown significantly this year, with important expansions of all section of the Materials Cloud, new AiiDA releases, new open source codes. We have put special effort towards ensuring the long-term sustainability of these resources beyond the NCCR, for example by starting the Learning Hub for Modelling and Simulation (Lhumos) platform, that will be the successor to the Material Cloud *Learn* section. Our strong commitment to open science was also acknowledged with a special mention (to Nicola Marzari's group) at the Swiss National Prize for Open Research Data.

We have continued our efforts for Equal Opportunities with more INSPIRE Potentials fellowships, several activities for girls and young women, Agility Plus funding, the participation in the #NCCRWomen campaign. We have created several education and training opportunities for young scientists and students, including a very successful MARVEL junior retreat and the participation in international summer schools from Pavia to Berlin to Kigali. We have also continued communicating our research through the website and in social media, and organizing communication events with CECAM, with more to come in 2024.

2 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 and in rest of the report the actions that we have taken in response to these comments.

General impression

As in previous years, the review panel is very impressed by the high quality of the research produced by the NCCR. But as the NCCR Director reminded the audience in the first presentation, an NCCR is not only about excellent science, it is foremost about collaborative science that could not have happened without the consortium, and which has a long-term structural impact. It is already clear in year 9 that NCCR MARVEL has succeeded in these two aspects as well. On the one hand, the NCCR has manoeuvred the downsizing requested in phase III fruitfully and is now composed of members willing to carry-on MARVEL's vision beyond the end of NCCR funding. On the other hand, the core activities of the NCCR have been secured for the long term by positioning research groups at the Paul Scherrer Institute (PSI) and at the Swiss Federal Laboratories for Materials Science and Technology (Empa), and through continued tight collaboration with the Swiss National Supercomputing Centre (CSCS). Securing the legacy of a NCCR already in year 9 is impressive and the review panel highly praised the consortium for this achievement, as well as the leadership of the Director.

In terms of structure-related areas, the panel commends the portfolio of activities in terms of communication and outreach and the fact that NCCR MARVEL is a role model for open science in Switzerland and world-wide. The Psi-k conference organised in the summer of 2022 is also deemed a great success. Finally, the review panel is very fond of the INSPIRE Potentials Master's fellowships for women and pleased that they will be extended to allow research stays in NCCR MARVEL groups for other underrepresented groups in the field.

We thank the panel for this very positive assessment — we are actually delighted to announce that the general Psi-k conference will be held again at EPFL in August 2025, on the wake of the great enthusiasm (and outstanding organization by our program manager Patrick Mayor and the MARVEL team) following the previous one in August 2022, with 1300+ participants.

Scientific performance, collaborations and added value

Pillar 1

The review panel considers the work presented in the progress reports and at the annual review to be of high scientific quality. However, the panel noted that most of the reported work is on alloys, and almost none on MOFs, and asked the NCCR management on the status of the collaboration with the group of Professor Berend Smit. The NCCR Director replied that indeed Professor Smit has stepped back from engagement in NCCR MARVEL, as he is overwhelmed with other funding obligations. This gap is replaced by the new junior PIs Michael Herbst and Anirudh Raju Natarajan, and the decision for this disassociation was supported by the Steering committee. The panel understands the situation, but also regrets it since the work on MOFs was the closest to market opportunity. Nevertheless, this is a natural progression, and the reviewers are pleased to hear that the new PIs are being so well integrated and already benefit from the network.

This is well understood, but it is also the mark of the great success for the vision of the proposal, with other senior PIs moving on to coordinate major activities in the field (e.g., see Matthias Troyer and Microsoft Quantum, Anatole von Lilienfeld and the Acceleration Consortium at the University of Toronto, Antoine Georges directing the Center for Computational Quantum Physics at the Flatiron, Michele Parrinello leading the Molecular Simulations group at the Italian Institute of Technology); and the work of Berend Smit on large-language models and younger former MARVEL researchers like Kevin Jablonka and

Philippe Schwaller promises also to be pioneering in the field. Most importantly, there is a new generation of junior professors that has entered the Swiss scientific environment and that is building powerful synergies with the goals of the project, thus laying also the foundation for longer-term collaborations and interactions that fulfill the promise of structural impact and goals.

Pillar 2

Overall, the reviewers commented that the machine learning (ML) landscape is very large and that the presented examples were interesting, but that they failed to see what MARVEL's niche is. They recommend showing the uniqueness of MARVEL's activities more prominently. They further asked about the value of ML in this field and were satisfied to hear that the intention is to go toward more accuracy for pragmatic applications, especially in the density functional theory (DFT) accuracy.

Indeed, this will be one of the clear challenges for Pillar 2, i.e., how to make the M-stack infrastructure usable and used by the different groups. One important element has been the embedding and long-term employment of Guillaume Fraux from the Ceriotti group into a permanent position in SCITAS at EPFL (the scientific IT group), initially supported for 2 years by MARVEL, and ensuring that the ML and data analytics capabilities are going to be supported in the long-term.

The panel is pleased to hear about the software trainings for students. However, similarly as mentioned above, they understand that the transfer towards the industry only works if the companies have research units and use Python.

We are actually very pleased about the interactions with industry. It has become clear that one of the core mechanisms for IP transfer in industry is actually that that concerns the hires and moves of MARVEL-trained personnel, with many now having leading roles in industry. Just a few examples could be those of the students/postdocs hired by Microsoft Quantum (Sebastiaan Huber, Leopold Talirz, Conrad Johnston, Loris Ercole, and Andrea Cepellotti), by Sandip De at BASF or Maximilian Amsler at Bosch. This is on one hand the best guarantee of long-term success and integration, but showcases also the excellent job opportunities for our own researchers (not to mention those that moved to academic institutions, as, e.g., Bingqing Chen now at UC Berkeley). At the same time, funding and close collaborations with both national and international industries continues strongly, often saturating our capabilities.

Pillar 3

The experts are very impressed by this pillar and mostly wondered about the data management plans, the quality of the data uploaded and the reproducibility. They were very pleased to hear that the Materials Cloud Archive *follows the FAIR principles (and is recommended by the SNSF as a FAIR repository), and that they have a solid protocol in place for the* $\sim$ *600 submissions per year. The panel members also report that the platforms and tools developed by the NCCR are being used by the international community, including themselves.*

We thank the review panel for the kind words; we see the remaining challenge as one of usability and user-friendliness of the AiiDA platform, and that will be one of the core efforts for the remaining time.

Pillar 4

The review panel is very impressed and satisfied that the arrangements for the legacy of NCCR MARVEL are already secured. The fact that PSI and Empa will be hosting the software, and that the respective teams are in place to take care of its curation, is applauded. At first, the panel was slightly surprised that the legacy of NCCR MARVEL would not be at EPFL, who is also currently hosting the Centre Européen de Calcul Atomique et Moléculaire (CECAM), but ultimately agreed that national laboratories are indeed a better option to perennialize the NCCR's activities. Scientific software needs to be maintained and curated by personnel hired for the long term, which is rarely the case at universities.

Indeed, we believe that while the intellectual legacy is in the form of new professors and new ideas in the field of MARVEL, the structural legacy needs to take place within the context of national laboratories and the establishment of "digital infrastructures" complementing the physical ones.

Further, the experts appreciate the Director's statement that MARVEL's legacy also lies in its current members and PIs, who will continue to work on the research topics at the core of the NCCR after its end. This attitude illustrates the great leadership of the Director, who is able to attract, motivate and promote young PIs. The panel also recognises that this

whole pillar shows the dedication and great vision of the Director for computational material science.

ASM

The panel congratulates the researchers in this project for their solid scientific work and for the high level of collaborations between EPFL, PSI, the University of Fribourg, Empa and ETHZ. However, at this point it seems disconnected to the other pillars and the reviewers hope to see more convergence in the coming years.

A core goal for the project is to develop the horizontal capabilities for materials and devices — from non-equilibrium Green's function methods to DMFT to device simulations — and so the interactions within the groups there are key, and are where we focused the effort. The relevance of this is also seen in new simulations pillars involving the PIs becoming now significant components in the current call for new 2026-onwards NCCR proposals.

Bonus project, QS

The only recommendation of the review panel regarding the full proposal was about the integration of this project with the rest of the NCCR's activities. Unfortunately, the links to the NCCR remain weak, and the synergies and collaborations are not yet visible.
The reviewers understand that the NCCR wanted to take on this very topical subject as an option for following latest developments in the field. If successful, this could indeed have a very significant impact. However, the panel believes that the researchers should move away from toy problems and asks for the validation on more complex applications, such as the ones that would be posed by the industry and in real settings. Even if it is not successful, there would be much to learn from these attempts. The reviewers also realise that this criticism can be applied to the whole worldwide community, yet strongly encourages the NCCR to try and go beyond the comfort zone.

Similarly to the previous project, we think that the most important goal is to make sure that the different PIs within the project create and sustain core collaborations in this field. Question 6 from the Executive summary aims to focus the effort on relevance to the real wold.

Agility Plus

Two of the four Agility Plus projects grantees presented their results during the annual review and both mentioned that the scheme was excellent seed financing to support curiosity-driven research. The initial idea of these experimental projects was that they would provide concrete (and surprising, as it turned out) cases to theorists and modellers in the NCCR. While the panel supports this initiative to promote women, it is unclear what will happen with the results of these projects and how well the recipients were included.
The reviewers are therefore slightly hesitant about the benefits of this measure for the female researchers and the consortium. At the same time, they also understand that continuing collaborations is difficult when people move away or have other priorities.

A positive note is that Ana Akrap is moving to a full professorship at the University of Zagreb. That MARVEL was actively instrumental in making sure she could be supported until the end of the school year in Fribourg is an example of the multiple avenues of support we deploy. Also, core priorities have been the full deployment of automated XPS/XAS capabilities, driven indeed by the needs, among others, from the project of Emiliana Fabbri, and of spin-orbit extension to the Koopmans functionals, driven by the project of Ana Akrap on $EuCd_2As_2$. Broadly speaking, we remain in need to attract more women scientists to the field (the challenge is particularly severe in the theory/computational field of MARVEL, but we reiterate here the inclusion of Sara Bonella, Zoë Holmes, and Lenka Zdeborová in the project); for this reason, we are particularly pleased that we were able to also replicate our initiative on "Women in Materias" with leading portraits at the entrance of the Institute of Materials at EPFL, to Mathematics, Physics, and Chemistry — showcasing role models is a key measure that we have always advocated.

Structure-related areas

Education and training

Several action items have taken place following the recommendation of the panel.

- The MARVEL junior retreat was restarted and a first one took place in Davos in September 2023, with great success (see section 5.1 on Education & Training for the details). Motivated students have already announced their intention to organize the next one in 2024.
- The 2023 junior retreat focused on building bridges, in particular between industry and academia. As mentioned in sec-

tion 5.1 on Education & Training, the workshop aimed to facilitate discussions, enabling participants to explore the practical applications of research and forge partnerships that bridge theory with real-world impact.

- We have been meeting with Kathryn Hess Bellwald, Associate Vice President for Student Affairs and Outreach to search for support of the summer camp for high-school students; she will investigate this through philanthropy at EPFL.
- The question of teaching credit was addressed through a meeting with Annalisa Buffa, Associate Vice President for Postgraduate education. Now, the doctoral schools do not intervene in the teaching load of doctoral students, and there is no general rule at EPFL regarding teaching credits. We need thus to deal case by case with each institute, and a request to the doctoral school in Materials has been put forward.

Equal opportunities

The review panel agrees that the NCCR can show real successes in this area after 9 years. The numbers speak for themselves and there seems to have been a clear increase in the number of female PhD students since phase I.
The panel strongly hopes that [the INSPIRE Potentials] fellowships will continue post NCCR funding and that EPFL will make them part of the school programs.

As mentioned we had a first contact with Kathryn Hess Bellwald, Associate Vice President for Student Affairs and Outreach also about this topic, and will seek support through philanthropy at EPFL. Another alternative is to have these fellowships directly funded through the faculty involved, given the fact that they represent also excellent opportunities to attract prospective future PhD students.

The review panel was also very pleased to see the creation of fellowships for under-represented groups, the various activities proposed to younger girls with at least 50% of the spots reserved for them and the efforts to promote a healthy work-life balance, such as the popular childcare offer at the Psi-k 2022 conference.

The creation of fellowships for under-represented groups hit some legal restrictions that are complex work in progress (in the Canton Vaud, visiting PhD students cannot get more than CHF 2'500 per month from all sources, that is half of what the wage of a PhD student is here); a higher wage is currently not possible (see more details in section 5.3 on Equal Opportunities).

Communication and outreach

The activities in this domain remain solid at the beginning of phase III. The highlights, news and portraits section on the website are well done and interesting.

The arrival of Nicola Nosengo has also provided a major boost the activities in this area.

Open science

This domain is a strength of the NCCR because it has been part of the core vision since the beginning. MARVEL has been a pioneer in the Swiss research landscape (and worldwide) and a model for the other NCCRs for open science and open access by providing a digital infrastructure of open simulations and data. The goal for the coming years is to go beyond FAIR data to FAIR simulations, which the panel applauds.

We thank the panel for the very kind words.

The reviewers are pleased that 96% of MARVEL papers are open access without embargo. The ones that are not, are in the field of chemistry, where the community is more resistant to the issue of open science and therefore where there are only very few open access journals. The NCCR is further very diligent in publishing their datasets, mainly on the Materials Cloud Archive, *which the SNSF recognises to be a FAIR repository since 2022.*

NCCR MARVEL also combined efforts with 6 other NCCRs to provide three 1-day open research data meetings in Zurich, Lausanne and Basel, which is considered a fantastic initiative by the review panel.

This was indeed a very fruitful collaboration with other NCCRs and the MARVEL scientific manager was very involved in the organization. More details on these can be found in the section 5.5 on Open Science.

Knowledge and Technology Transfer (KTT)

In terms of knowledge transfer, the NCCR stands very successful in this 9th year. The long-term fate of the data and the developed open science software has been secured at PSI. The panel commented that

this is usually where the big projects in the field have failed, and MARVEL managed to do what many dreamt about.
The organization of the Psi-k 2022 conference is another great success of the NCCR in the past year according to the reviewers, where the whole community met in Lausanne. The panel salutes the actions put in place for the under-represented groups, such as fellowships for scientists based in Africa or for refugees.

Again, we thank the panel for the very kind words.

The NCCR continues to have a number of successful collaborations with industry, but the transfer of technology occurs mostly when companies hire MARVEL researchers. As a matter of fact, unless someone at a company is already familiar with Python and/or the MARVEL software, the uptake has been difficult, which the panel understands and relates to. Nevertheless, it is important to keep the dialogue open and the reviewers recommend that in the coming years, Empa, with its industry contact, could organize an "industry day". This event, along with the training on collaborating with the industry and IP rights mentioned in chapter 5.1, could represent great opportunities for the junior researchers.

Two action items are also planned for 2024, with an industry day at Empa, to continue the dialogue with industry, and a dedicated session on IP rights, at the next 2024 junior retreat. In passing, we note that both at the September 2023 junior retreat, and at the January 2024 general retreat, we had sessions specifically dedicated to interactions with and experiences in industry.

Structural aspects and long-term plans

Support by the Home Institution

The panel is pleased to see that the NCCR is exploiting the full potential of these hires and managed to attract these professors within its ranks.

Integration in other federal research institutions

As mentioned regarding Pillar 4, the review panel is very impressed by the already settled legacy plans of the NCCRs. With personnel and activities anchored at PSI, Empa and CSCS, the NCCR has already had a long-term impact on the Swiss research landscape. During the annual review, the deputy director of CSCS presented their plans for HPC and the link with NCCR MARVEL. The panel is glad to hear that CSCS consider MARVEL to be a role model and that this collaboration is a beneficial learning experience, which allows them to building computing infrastructures for scientific communities. Through its links with PSI, CSCS will stay in close contact with the MARVEL legacy.

Indeed, we thank the panel for these words; these points, both on the support by the Home Institution and the integration in other federal research institutions, are also elaborated in Chapters 6 and 7 of this report.

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

Research

To follow up on the phase II Agility Plus projects in order to foster continuity and absorption of the grantees. There is an opportunity to address the challenges demonstrated in the two high-lighted experimental Agility projects by exploiting the computational and theoretical competence within MARVEL.

As mentioned, Ana Akrap and Emiliana Fabbri are associated to Pillar 4, and we are focusing some of the computational efforts to support their experimental research. In addition, Ana Akrap's salary will be half-supported by MARVEL in the spring 2024, to allow her to stay at UniFR until the end of the school year for her children, before a move to the University of Zagreb as a full professor. Sereina Riniker (as a computational PI) is still in the list of host-laboratories for the INSPIRE Potentials fellowships and is presently hosting one such student (Eva Doloszeski); in addition, Laura Grigori, a new professor at EPFL and PSI and an applied mathematician, has also become a host for future INSPIRE Potentials fellowships.

To strive for demonstrating the use of the developed methods and showcase their predictive capabilities on real-world or experimental challenges.

Indeed, examples will be shown at the site visit of these efforts taking place both with industry and with experimental facilities.

To bring the Bonus and the Advanced Simulation Methods projects to converge with the goals and activities of the pillars.

As discussed, this will also be presented at the site visit.

Structure-related areas

To continue the dialogue with the industry, even if it is difficult and the uptake is limited. Empa could organise activities/events that engage the industry, such as an industry day.

This is very active, with events at all retreats and an industry day planned at Empa.

To reinstall the junior retreats for PhD students and postdocs and include sessions on entrepreneurship, IP rights and technology transfer sessions.

This is also done, first in September 2023, with great success, and will be repeated further.

Recommendation to the Home Institution

In terms of legacy, EPFL should invest in continuing the INSPIRE Potentials fellowships scheme and the summer camp for high school students. It would be important to offer appropriate teaching credit for the (PhD) students involved in these activities.

The different philanthropy channels are being explored, but one possibility for the INSPIRE Potentials fellowships is also to preserve these with funding directly from the PIs involved.

3 NCCR Organisation

3.1 Structure and organisation of the NCCR, management activities

3.1.1 Structure and organisation of the NCCR

In phase III, MARVEL's mission revolves around six core activities, spread over six projects, as represented in Fig. 1. In year 10 the structure of the NCCR is unchanged compared to year 9. The composition of the bodies (Directorate, Executive Committee, and Scientific Committee) is also unchanged.

With the new phase, the composition of the Scientific and the Industrial Advisory boards have been slightly revised. The Scientific Advisory Board (SAB) is still chaired by Giulia Galli (Univ. Chicago). Gian-Luca Bona retired and was replaced by Tanja Zimmermann, the new director of Empa. Ignacio Pagonabarraga has completed his term as director of CECAM and was replaced by his successor, Andrea Cavalli. Risto Nieminen (Aalto Univ.) and Alexander Lichtenstein (Univ. Hamburg) left and Peter Haynes (Imperial College, chair of Psi-k's board of trustees) has stepped in. Finally, Gabriel Aeppli (PSI), Karsten Jacobsen (Technical Univ. Denmark, Lyngby), Boris Kozinsky (Harvard Univ.) and Sadasivan Shankar (Stanford Univ.) continue to serve on the SAB. The composition of the Industrial Advisory Board (IAB) was also adjusted. Still chaired by Erich Wimmer (Materials Design), the board welcomes Paola Gori Giorgi (Microsoft Research AI4Science) as a newcomer. The other members (unchanged) are Nicolas Cudré-Mauroux (previously Solvay, from 2024 SICPA), Thomas

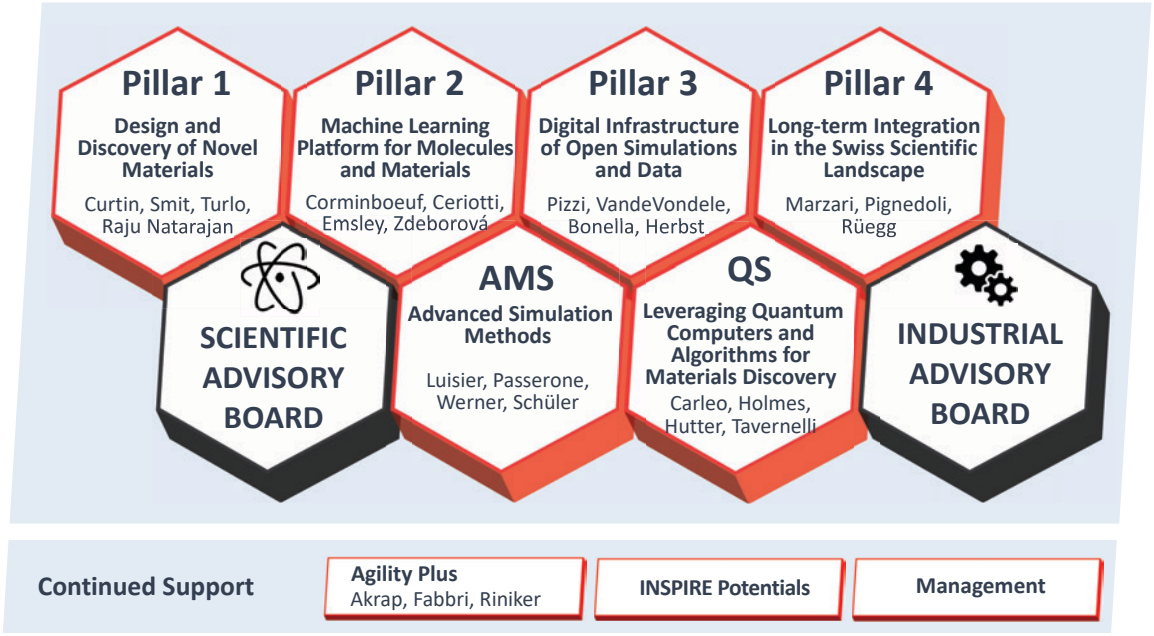

Figure 1: *Organization of MARVEL in phase III.*

Eckl (Robert Bosch), and Arnaud Grandeury (Novartis). Frédéric Diologent (Richemont) and Ryoji Asahi (formerly Toyota, moved to academia) have left the board. Some members of both boards were present at the MARVEL Review and Retreat in Grindelwald in January 2024.

3.1.2 Management activities

Events organisation

In year 10, since February 2023, MARVEL management organized the meetings, lectures and events described in chapter 5. We mention here, for example:

- MARVEL site visit, EPFL, March 28–29.
- MARVEL stand at EPFL Open Days 2023, April 29–30.
- NCCRWomen stand at EPFL Open Days 2023, April 29–30.
- 3 NCCR Open Research Data Meetings in Zurich, April 28, Lausanne, May 8, and Basel, June 2, particularly involved in the Lausanne one.
- Summer camp for high school students *Des atomes aux ordinateurs, à la découverte de la programmation scientifique*, EPFL, June 26–30.
- MARVEL lab visit for girls participating to the summer camp "Matériaux super géniaux", EPFL, August 18.
- MARVEL Junior Retreat 2023, Davos, September 12–15.
- CECAM-MARVEL Classics in molecular and materials modelling, Eberhard Gross (Hebrew Univ. Jerusalem) and Angel Rubio (MPSD), EPFL and online, September 28.
- 6 online projects meetings (Pillars 1 to 4, ASM and QS), September-October.
- MARVEL Communication open mic session, EPFL and online, October 3.
- INSPIRE Potentials networking event, EPFL, October 19.
- EPFL Information days for high-school students, visit of labs, EPFL, November 23.
- NCCRs gathering event, EPFL, December 4.
- MARVEL Review and Retreat, Grindelwald, January 17–19, 2024.
- BIG-MAP EUnified Battery Data Space Workshop, Grindelwald, January 29–31, 2024.
- INSPIRE Potentials — MARVEL Master's Fellowships for female Master's students, with 2 calls in April and October.
- 2 weeks of #NCCRWomen portraits on social networks, February 13–17 and March 27–31.
- 3 online MARVEL distinguished lectures, Kristian Sommer Thygesen (DTU), March 23, Claudia Felser (MPI CPfS, Dresden), May 2, and Emmanouil Kioupakis (Univ. Michigan), June 20.
- 7 hybrid junior seminars, EPFL and online, from February to December, with pizza served before or after.
- 4 seminars at EPFL or hybrid (Michael Herbst (EPFL), Vojtech Vlcek (UCSB), Zhiting Tian (Cornell), Andrew Briggs (Oxford)).
- 5 online or hybrid Executive Committee meetings.

Other events

In addition, in year 10, MARVEL members organized at least 14 conferences, tutorials or workshops, either in person or online; MARVEL sponsored 4 of these.

Measures

MARVEL has prepared an updated version of its internal regulations for phase III. It was signed by all parties in June 2023.

3.2 Changes to the consortium's composition

Three new PIs entered MARVEL in May 2023.

- Zoë Holmes (newly hired at EPFL in August 2022) joined the Quantum Simulation project.
- Lyndon Emsley (EPFL), already part of MARVEL for the last two years of phase II, joined Pillar 2 to continue the collaboration started then.
- Michael Herbst was hired at EPFL thanks to a proposal conceived by Assyr Abdulle (EPFL Math) and Nicola Marzari and submitted to the EPFL leadership for a joint interfaculty chair in Math and Materials, and started in March 2023.

The funding for Zoë Holmes derived from half the funding planned for Agility Plus projects in phase III. The other half was allocated to Sara Bonella (EPFL) to increase her MARVEL research funding. The funding of both Lyndon Emsley and Michael Herbst was made possible through the reallocation of part of the funding of Pillar 1, with the departure of both Bill Curtin and Berend Smit for the second half of the phase. Indeed, Berend Smit has left the consortium at the end of 2023. Bill Curtin has officially retired from EPFL on December 31, 2022 and has returned to the USA. During year 10, he could still maintain a team at EPFL and hire a few people through MARVEL funding. He

will leave the consortium at the end of year 10 on April 30, 2024. Anirudh Raju Natarajan will take the lead of Pillar 1.
On the management side, Carey Sargent (20%) left her role in the written communication for the website and the social media. She was replaced in this task by Nicola Nosengo, who is also chief editor of *Nature* Italy. Previously, Nicola Nosengo was also for a few years a science writer for the NCCR Robotics. The rest of the MARVEL management team is unchanged.

4 Research

4.1 Status of collaboration / integration and added value

We start this section with a reminder on how timely and fitting the broad topic of the NCCR is, at a time when even major companies — from Microsoft to Google/DeepMind — broadly publicize their efforts and plans in materials discovery. And it is actually reassuring that, at a time when major funding efforts are decided at the policy-making level, the SNSF focuses on investing in long-term projects that are internationally reviewed and screened by communities of scientists.

4.1.1 Status of collaborations and integration

At the NCCR level

Key collaborations have taken place that would not have happened without MARVEL; these include the efforts of Pillar 1 (Curtin/Raju Natarajan/Turlo), Pillar 2 (Corminboeuf/Ceriotti), Pillar 3 (MaZe and SIRIUS), Pillar 4 (PSI and Empa), and Advanced Simulation Methods (Luisier/Passerone, and Passerone/Werner). These are complemented by a very fitting project on quantum computing meshing academic and industrial leadership in the field, with established MARVEL researchers (Carleo/Tavernelli/Hutter). Also, new members on the algorithmic side have found a natural place in the project: Herbst in Pillar 3, Schüler in Advanced Simulation Methods, and Holmes in Quantum Simulations.

At the national level

The key platform players of phase I (PSI, Empa, CSCS) have been not only close partners for the entire duration of MARVEL, but have enabled to transition the center to the post-2026 landscape. This includes the creation of the Scientific Computing, Theory and Data division at PSI, where, in additional to the creation of the Laboratory for Materials Simulations, two other major efforts and hires between PSI and EPFL took place, with the appointment of Prof. Laura Griogori to lead the Laboratory of Simulation and Modeling, and Prof. Andrea Läuchli to lead the Laboratory for Theoretical and Computational Physics. Also, the computational activities at Empa are now integrated in the Scientific IT division there.

At the international level

Core partners have been MaX, the EU Centre of Excellence for e-infrastructure on Materials Design at the eXascale (2015–2026 or longer), and BIG-MAP, the EU flagship initiative for Battery2030+. MaX has consistently shared the objectives of MARVEL, and has been a key partner in the development of the Materials Cloud services (including the federation of the *Archive* with CINECA and Jülich), deployment of exascale-ready codes (including QUANTUM ESPRESSO and SIRIUS), and of data analytics. MaX partners have been instrumental in making the AiiDA Common Workflows project into a broad community effort. BIG-MAP, involving 34 institutions, is also a key partner — the internal BIG-MAP Archive is modeled on the Materials Cloud *Archive*, and is now being finalized to push automatically data on the Materials Cloud when they become open access, while also being deployed across all the Battery2030+ projects. Also, BIG-MAP has been an enthusiastic promoter of the MARVEL plan of externalizable capabilities (either experimental or computational) that can be driven or interrogated through common user interfaces.

4.1.2 Added value

The MARVEL hires of Anirudh Raju Natarajan at EPFL and Michael Schüler at PSI, together with the arrivals of Giuseppe Carleo, Zoë Holmes, and Michael Herbst at EPFL ensure that a new generation of researchers in the field will be present in Switzerland and at EPFL.

4.2 Results from year 10

Pillar 1 — Design and Discovery of Novel Materials

Project leaders: William Curtin (EPFL), **Berend Smit** (EPFL)

Partners: Anirudh Raju Natarajan (EPFL), **Vladyslav Turlo** (Empa), Michele Ceriotti (EPFL)

1 Progress of the different efforts

1.1 Metal alloys

The effort in metal alloys has seen significant achievements and progress in the past year spanning high entropy alloys, lightweight metals, and alloy systems of interest to Empa. Only some major collaborative efforts are highlighted here. Project work in additive manufacturing is ongoing and will be discussed in a future report.

With our previous computational discovery of the Hf-Mo-Nb-Ti alloy family as promising for a combination of high temperature strength and room temperature ductility [1], Natarajan and Curtin have applied the cluster expansion (CE) method to make first-principles predictions of the phase behavior over the entire composition range while considering BCC, B2, HCP, and C15 phases. The desired solid solution state for compositions of interest is stable at 1'200°C (Fig. 1a), while the Hf-Mo interactions dominate and drive short-range ordering (SRO) at relevant temperatures (Fig. 1b). We have also demonstrated the accuracy of Vegard's law for estimating solute misfit volumes that enter the strength theory. More broadly, Curtin has completed the modeling of strengthening in the presence of SRO and developed easily-usable analytical and graphical results applicable to fcc and bcc alloys of any composition [2]. A key unexpected result is that SRO can decrease the dominant "misfit" strengthening in certain common situation. This unexpected result has been further demonstrated by targeted atomistic simulations in model bcc alloys [3]. We are now combining the SRO, CE, misfit volumes, and analytical models to make detailed predictions of strengthening in selected Hf-Mo-Nb-Ti alloys.

Parallel efforts by Natarajan have focused on exploring alloy chemistries that can enhance the strength of refractory high-entropy alloys through precipitation hardening. Utilizing a cluster expansion model parameterized from first-principles calculations, we employed Monte Carlo simulations to investigate the high-temperature behavior of a senary Al-Nb-Ta-Ti-V-Zr alloy. Finite-temperature phase stability, as estimated from our model, indi-

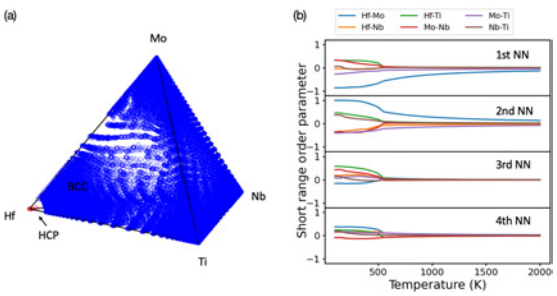

Figure 1: *(a) Phase diagram of quarternary Hf-Mo_Nb-Ti at 1'200°C showing solid solutions in the high-entropy regime. (b) Warren-Cowley short-range-order parameters for all solute pairs in $Hf_{15}Mo_{20}Nb_{30}Ti_{35}$ versus temperature, showing Hf-Mo ordering to dominate.*

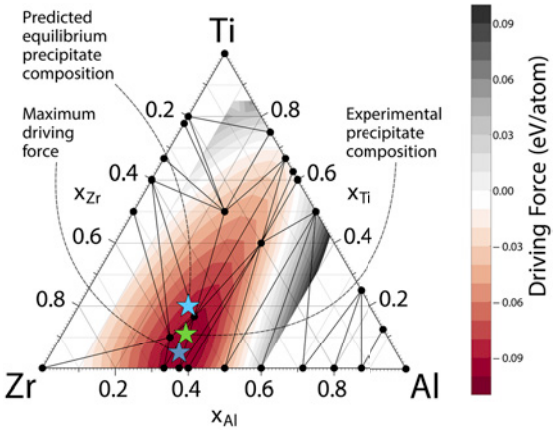

Figure 2: *Precipitate compositions and driving forces as predicted at 600°C by a cluster expansion model and Monte Carlo simulations in a senary Al-Nb-Ta-Ti-V-Zr alloy.*

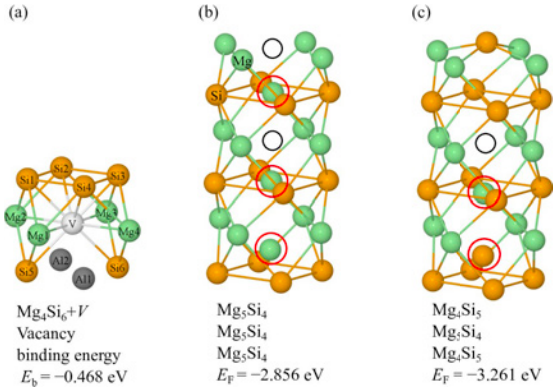

Figure 3: *(a) Vacancy strongly trapped inside a 10-atom Mg-Si cluster; (b) pre-β″ and (c) pre-β″ with Si capping top and bottom, with significantly lower formation energy.*

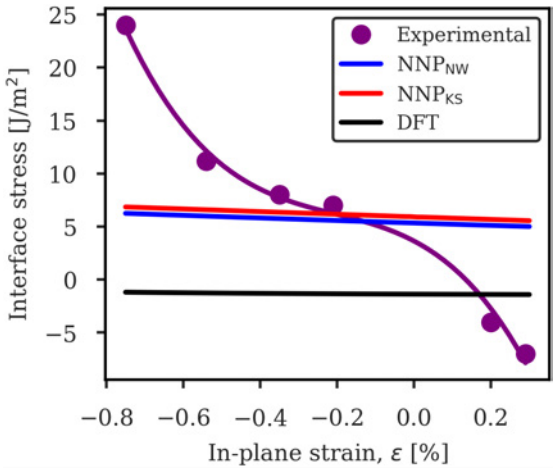

Figure 4: *Interface stresses in the Cu/W nano-multilayers obtained with the NNP, DFT, and experimental results for the respective interfaces, for the experimental strain range.*

cates the emergence of an ordered precipitate from the disordered phase over a broad composition range. Our predictions for precipitate composition and phase fractions are in excellent agreement with recent experimental findings (Fig. 2). We find that the emergence of ordered phases in this alloy is driven by the strong segregation of aluminum to a single sublattice of the B2 structure. Surprisingly, our results reveal that despite conventional B2 orderings being mechanically and thermodynamically unstable in this system, defect orderings on B2 emerge as metastable states. Further research will focus on searching for alloying elements that can enhance the thermal stability of the precipitate phase.

In lightweight metals, Curtin and Ceriotti have completed the analysis of clustering and vacancy trapping in the technologically-important Al-6xxx (Al-Mg-Si) alloys using their neural-network potential (NNP) [4]. We have demonstrated the long-held belief that vacancies are strongly trapped in small (10-14 atom) Si-Mg clusters, thus halting natural aging process (Fig. 3a). Our analysis has also uncovered the existence of energetically stable clusters where Si replaces Mg on capping sites of needle-like pre-β'' clusters (Fig. 3, b and c), rationalizing experimental evidence that natural aged clusters must be partially dissolved before nucleation of β'' precipitates can proceed during artificial aging. In Mg, Curtin has used our previous Mg NNP to demonstrate (i) a low-temperature ($T < 150$ K) instability in prismatic slip [5] and (ii) a new 3D mechanism for thermally-activated prismatic slip at high temperatures ($T > 150$ K) [6], both capturing long-standing and previously-perplexing experimental results.

We have continued to develop NNPs for other metallurgical applications. Turlo and Curtin have developed an NNP for the Cu-W system. This has enabled better interpretation of experimental measurements of interface stress in relation to internal strains in Cu/W nano-multilayers (solid circles in Fig. 4). Density functional theory (DFT) calculations for the generic Cu/W interface (the only one feasible for small supercells) and NNP calculations for textured Kurdjumov-Sachs and Nishiyama-Wassermann interfaces demonstrate that the experimental measurements do not correspond to the variation of interface stress with residual in-plane strains in the multilayers (which is rather weak), but to the different nature of the interfaces, i.e. generic/random vs textured. Further research will be focused on identifying the nature of interfaces with the highest interface stress, with the main hypothesis that it is a premixed amorphous structure. A more-refined NNP to enable such calculations is near completion (Liyanage *et al.*, in preparation), and its applications to this and other challenges at Empa are in progress. Following earlier development of an NNP for hcp Zr, Curtin has also created an excellent potential for Zr-H (Liyanage *et al.*, in preparation), since hydride formation in nuclear applications of Zr is a component-critical issue. The potential accurately captures the energetics of various competing hydride phases, their surface energies, and their fracture behavior, in addition to H interstitials in Zr and improved performance of pure Zr itself.

1.2 Metal-Organic Frameworks

The effort in metal-organic frameworks has achieved two important goals. The first achievement is the successful development of a methodology to predict whether a covalent organic framework (COF) is a candidate for photocatalysis [7]. The second achievement is an understanding of the effect of adding Zn-MOF-74 to the cobalt-catalyzed hydroformylation of 1-hexene. In addition, we have co-organized a hackathon in which we illustrated the use of large language models in chemistry [8, 9].

Covalent organic frameworks (COFs) stand out as prospective organic-based photocatalysts, given their intriguing optoelectronic properties, such as visible light absorption and high charge-carrier mobility. The "Clean, Uniform, Refined with Automatic Tracking from Experimental Database"(CURATED) COFs [10] is a database of reported experimental COFs that until now remained mostly unexplored for photocatalysis. In this study, the CURATED COFs database is screened for discovering potential photocatalysts using a set of DFT-based descriptors that cost-effectively assess visible light absorption, preliminary thermodynamic feasibility of the desired pair of redox reactions, charge separation, and charge-carrier mobility. The workflow (Fig. 5) can shortlist 13 COFs as prospective candidates for water splitting and identify materials (Nx-COF (x = 0–3)) that have been reported as candidates for hydrogen evolution reaction. Overall, the strategy addresses the challenge of exploring many COFs by directing future research toward a selective group of COFs while providing valuable insights into the structural design for achieving a desired photocatalytic process.

The tandem hydroformylation-aldol condensation (tandem HF-AC) reaction offers an efficient synthetic route to synthesizing industrially relevant products. The addition of Zn-MOF-74 to the cobalt-catalyzed hydroformylation of 1-hexene enables tandem HF-AC under milder pressure and temperature conditions than the aldox process, where zinc salts are added to cobalt-catalyzed hydroformylation reactions to promote aldol condensation. The yield of the aldol condensation products increases by up to 17 times compared to that of the homogeneous reaction without MOF and up to 5 times compared to the aldox catalytic system. Both $Co_2(CO)_8$ and Zn-MOF-74 are required to enhance the activity of the catalytic system significantly. Density functional theory simulations and Fourier-transform infrared experiments show that heptanal, the product of hydroformylation, adsorbs on the

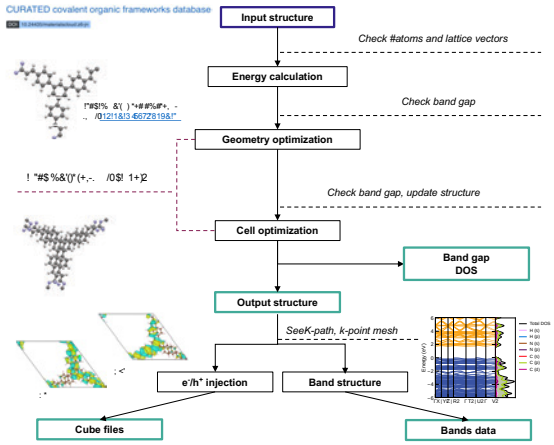

Figure 5: *Flowchart of the workflow developed for this screening study. It takes as input the structures from the CURATED COFs database (box highlighted in Persian indigo) and then checks the number of atoms and lattice parameters. The next step is a single-point energy calculation. The structure is optimized if this calculation confirms that we have a closed-shell system with a semiconducting band. From the optimized structure, the workflow computes the main outputs (boxes highlighted in jungle green) utilized to calculate our photocatalytic DFT descriptors, namely, band gap and band alignment (with band gap and cube files printed after optimization), charge separation (with cube files from electron and hole injection) and charge carrier effective masses (with bands data).*

open metal site (OMS) of Zn-MOF-74, thereby increasing the electrophilic character of the carbonyl carbon atom and facilitating the condensation [11].

Large-language models (LLMs) such as GPT-4 caught the interest of many scientists. Recent studies suggested these models could be useful in chemistry and materials science. To explore these possibilities, we organized a hackathon. Participants employed LLMs for various applications, including predicting properties of molecules and materials, designing novel tool interfaces, extracting knowledge from unstructured data, and developing new educational applications. The diverse topics and the fact that working prototypes could be generated in less than two days highlight that LLMs will profoundly impact the future of our fields. The rich collection of ideas and projects also indicates that the applications of LLMs are not limited to materials science and chemistry but offer potential benefits to a wide range of scientific disciplines [8, 9].

2 Contribution to overall goals and initial proposal

The project continues to achieve major goals that were laid out in the phase III proposal while exploiting opportunities to resolve important and open questions in the field as we have new insights. The PIs continue to be at the forefront of the field of high entropy alloys, lightweight metals, and metal-organic frameworks, providing new methods, new insights, and enabling the discovery of new promising materials.

3 Collaborative and interdisciplinary components

Internal MARVEL collaborations among the Pillar 1 members in the metallurgy thrust have been indicated above. We continue to have formal and informal collaborative interactions with external colleagues worldwide. The research remains within the broad domain of computational metallurgy, but within the domain encompasses the application of first principles methods, alloy thermodynamics, machine learning, atomistic simulations, and new mechanistic concepts and associated theories that (i) connect nanoscale behavior to macroscale performance and (ii) enable prediction of new alloys with enhanced mechanical performance.

The predictions of the adsorption thermodynamics of gasses in MOFs are part of the PrISMa platform, in which materials are ranked for their performance in carbon capture applications. The PrISMa platform involves the integration of the material's properties with process design, techno-economics, and life-cycle assessment [12].

MARVEL publications

List of publications either resulting directly from the NCCR (marked with a red hexagon) or with minor contributions from the NCCR.

- [1] Y. Rao, C. Baruffi, A. D. Luca, C. Leinenbach, and W. A. Curtin, *Theory-guided design of high-strength, high-melting point, ductile, low-density, single-phase BCC high entropy alloys*, Acta Materialia **237**, 118132 (2022).
- [2] S. Nag and W. A. Curtin, *Solute-strengthening in metal alloys with short-range order*, Acta Materialia **263**, 119472 (2024).
- [3] X. Liu and W. Curtin, *Atomistic simulations reveal strength reductions due to short-range order in alloys*, Acta Materialia **263**, 119471 (2024).
- [4] A. C. P. Jain, M. Ceriotti, and W. A. Curtin, *Natural aging and vacancy trapping in Al-6xxx*, Journal of Materials Research **38**, 5171 (2023).
- [5] X. Liu, M. Rahbar Niazi, T. Liu, B. Yin, and W. A. Curtin, *A low-temperature prismatic slip instability in Mg understood using machine learning potentials*, Acta Materialia **243**, 118490 (2023).
- [6] X. Liu and W. Curtin, *Mechanism of thermally-activated prismatic slip in Mg*, Acta Materialia **262**, 119402 (2024).
- [7] B. Mourino, K. M. Jablonka, A. Ortega-Guerrero, and B. Smit, *In Search of Covalent Organic Framework Photocatalysts: A DFT-Based Screening Approach*, Advanced Functional Materials **33**, 2301594 (2023).
- [8] K. M. Jablonka, Q. Ai, A. Al-Feghali, S. Badhwar, J. D. Bocarsly, A. M. Bran, S. Bringuier, L. C. Brinson, K. Choudhary, D. Circi, S. Cox, W. A. de Jong, M. L. Evans, N. Gastellu, J. Genzling, M. V. Gil, A. K. Gupta, Z. Hong, A. Imran, S. Kruschwitz, A. Labarre, J. Lála, T. Liu, S. Ma, S. Majumdar, G. W. Merz, N. Moitessier, E. Moubarak, B. Mouriño, B. Pelkie, M. Pieler, M. C. Ramos, B. Ranković, S. G. Rodriques, J. N. Sanders, P. Schwaller, M. Schwarting, J. Shi, B. Smit, B. E. Smith, J. Van Herck, C. Völker, L. Ward, S. Warren, B. Weiser, S. Zhang, X. Zhang, G. A. Zia, A. Scourtas, K. J. Schmidt, I. Foster, A. D. White, and B. Blaiszik, *14 examples of how LLMs can transform materials science and chemistry: a reflection on a large language model hackathon*, Digital Discovery **2**, 1233 (2023).
- [9] K. M. Jablonka, P. Schwaller, A. Ortega-Guerrero, and B. Smit, *Leveraging Large Language Models for Predictive Chemistry*, ChemRxiv. Preprint., to be published in Nature Machine Intelligence (2024), doi:10.26434/chemrxiv-2023-fw8n4-v3.
- [10] D. Ongari, A. V. Yakutovich, L. Talirz, and B. Smit, *Building a Consistent and Reproducible Database for Adsorption Evaluation in Covalent-Organic Frameworks*, ACS Central Science **5**, 1663 (2019).
- [11] P. Gäumann, T. Rohrbach, L. Artiglia, D. Ongari, B. Smit, J. A. van Bokhoven, and M. Ranocchiari, *Tandem Hydroformylation-Aldol Condensation Reaction Enabled by Zn-MOF-74*, Chemistry–A European Journal **29**, e202300939 (2023).

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- [12] C. Charalambous, E. Moubarak, J. Schilling, E. Sanchez Fernandez, J.-Y. Wang, L. Herraiz, F. Mcilwaine, K. M. Jablonka, S. M. Moosavi, J. Van Herck, G. Mouchaham, C. Serre, A. Bardow, B. Smit, and S. Garcia, *Shedding Light on the Stakeholders' Perspectives for Carbon Capture*, ChemRxiv. Preprint. (2023), doi:10.26434/chemrxiv-2023-sn90q.

List of year 10 publications related to Pillar 1

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).

⬢○ X. Liu and W. Curtin
Mechanism of thermally-activated prismatic slip in Mg
Acta Materialia **262**, 119402 (2024).
Group(s): Curtin / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:bf-5x

⬢○ S. Nag and W. A. Curtin
Solute-strengthening in metal alloys with short-range order
Acta Materialia **263**, 119472 (2024).
Group(s): Curtin / Project(s): P1
Links to article: Journal / Open access
Related datasets: not applicable

⬢○ X. Liu and W. Curtin
Atomistic simulations reveal strength reductions due to short-range order in alloys
Acta Materialia **263**, 119471 (2024).
Group(s): Curtin / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:kz-b7

○ V. Eyert, J. Wormald, W. A. Curtin, and E. Wimmer
Machine-learned interatomic potentials: Recent developments and prospective applications
Journal of Materials Research **38**, 5079 (2023).
Group(s): Curtin / Project(s): P1
Links to article: Journal / Open access
Related datasets: not applicable (review article)

○ H. Gustafsson, M. Kozdra, B. Smit, S. Barthel, and A. Mace
Predicting Ion Diffusion from the Shape of Potential Energy Landscapes
Journal of Chemical Theory and Computation **20**, 18 (2023).
Group(s): Smit / Project(s): P1
Links to article: Journal / Open access
Related datasets: not applicable

⬢○ B. Yin, L. Li, S. Drescher, S. Seils, S. Nag, J. Freudenberger, and W. A. Curtin
Solute misfit and solute interaction effects on strengthening: A case study in AuNi
Acta Materialia **257**, 119118 (2023).
Group(s): Curtin / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:tn-jh

⬢○ M. R. Niazi and W. A. Curtin
Solute strengthening of edge prism dislocations in Mg alloys
European Journal of Mechanics - A/Solids (2023), doi:10.1016/j.euromechsol.2023.105128.
Group(s): Curtin / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:h2-x5

⬢○ J. F. Troncoso, Y. Hu, N. M. della Ventura, A. Sharma, X. Maeder, and V. Turlo
Machine learning of twin/matrix interfaces from local stress field
Computational Materials Science **228**, 112322 (2023).
Group(s): Turlo / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:aj-wq

⬢ S. Gramatte, L. P. H. Jeurgens, O. Politano, J. A. Simon Greminger, F. Baras, A. Xomalis, and V. Turlo
Atomistic Simulations of the Crystalline-to-Amorphous Transformation of γ–Al_2O_3 Nanoparticles: Delicate Interplay between Lattice Distortions, Stresses, and Space Charges
Langmuir **39**, 6301 (2023).
Group(s): Turlo / Project(s): P1
Links to article: Journal / Open access (embargo 25.04.2024)
Related datasets: not applicable (review article)

⬢○ G. Winkens, A. Kauffmann, J. Hermann, A. K. Czerny, S. Obert, S. Seils, T. Boll, C. Baruffi, Y. Rao, W. A. Curtin, R. Schwaiger, and M. Heilmaier
The influence of lattice misfit on screw and edge dislocation-controlled solid solution strengthening in Mo-Ti alloys
Communications Materials **4**, 26 (2023).
Group(s): Curtin / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.5445/IR/1000157205

A. C. P. Jain, M. Ceriotti, and W. A. Curtin
Natural aging and vacancy trapping in Al-6xxx
Journal of Materials Research **38**, 5171 (2023).
Group(s): Ceriotti, Curtin / Project(s): P1, P2
Links to article: Journal / Open access
Related datasets: not applicable

P. Gäumann, T. Rohrbach, L. Artiglia, D. Ongari, B. Smit, J. A. van Bokhoven, and M. Ranocchiari
Tandem Hydroformylation-Aldol Condensation Reaction Enabled by Zn-MOF-74
Chemistry–A European Journal **29**, e202300939 (2023).
Group(s): Smit / Project(s): P1
Links to article: Journal / Open access
Related datasets: not applicable

K. M. Jablonka, P. Schwaller, A. Ortega-Guerrero, and B. Smit
Leveraging Large Language Models for Predictive Chemistry
ChemRxiv. Preprint., to be published in Nature Machine Intelligence (2024), doi:10.26434/chemrxiv-2023-fw8n4-v3.
Group(s): Smit / Project(s): P1
Links to article: Journal / Open access
Related datasets: github.com/kjappelbaum/gptchem

K. M. Jablonka, Q. Ai, A. Al-Feghali, S. Badhwar, J. D. Bocarsly, A. M. Bran, S. Bringuier, L. C. Brinson, K. Choudhary, D. Circi, S. Cox, W. A. de Jong, M. L. Evans, N. Gastellu, J. Genzling, M. V. Gil, A. K. Gupta, Z. Hong, A. Imran, S. Kruschwitz, A. Labarre, J. Lála, T. Liu, S. Ma, S. Majumdar, G. W. Merz, N. Moitessier, E. Moubarak, B. Mouriño, B. Pelkie, M. Pieler, M. C. Ramos, B. Ranković, S. G. Rodriques, J. N. Sanders, P. Schwaller, M. Schwarting, J. Shi, B. Smit, B. E. Smith, J. Van Herck, C. Völker, L. Ward, S. Warren, B. Weiser, S. Zhang, X. Zhang, G. A. Zia, A. Scourtas, K. J. Schmidt, I. Foster, A. D. White, and B. Blaiszik
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Digital Discovery **2**, 1233 (2023).
Group(s): Smit / Project(s): P1
Links to article: Journal / Open access
Related datasets: not applicable (review article)

B. Mourino, K. M. Jablonka, A. Ortega-Guerrero, and B. Smit
In Search of Covalent Organic Framework Photocatalysts: A DFT-Based Screening Approach
Advanced Functional Materials **33**, 2301594 (2023).
Group(s): Smit / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.7590815

C. Baruffi, F. Maresca, and W. A. Curtin
Screw vs. edge dislocation strengthening in body-centered-cubic high entropy alloys and implications for guided alloy design
MRS Communications **12**, 1111 (2022).
Group(s): Curtin / Project(s): P1
Links to article: Journal / Open access
Related datasets: not applicable (no data)

J. F. Troncoso, G. Lorenzin, C. Cancellieri, and V. Turlo
Explaining the Effect of In-Plane Strain on Thermal Degradation Kinetics of Cu/W Nano-Multilayers
Acta Materialia, Inc. First Look (2023), doi:10.2139/ssrn.4575644.
Group(s): Turlo / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:ah-f4

Pillar 2 Machine Learning Platform for Molecules and Materials

Project leaders: Clémence Corminboeuf (EPFL), **Michele Ceriotti** (EPFL)

Partners: Lenka Zdeberová (EPFL), **Lyndon Emsley** (EPFL), Giuseppe Carleo (EPFL)

1 Progress of the different efforts

In 2023 this Pillar has made excellent progress along the lines set forward in the proposal, developing further the collaborations between the partner labs. The efforts to develop a modular software platform for atomistic machine learning (M-stack) have reached an important milestone with a first version of a torchscript compatible model based on the Metatensor library, as well as with preliminary integration of the libraries to compute density-correlation descriptors with Q-stack and NetKet. High-quality documentation, and tutorials to showcase typical use cases improve the usability of M-stack. At the same time, we have pushed ahead with the study of the fundamental nature of machine learning (ML) models, with the integration of ML and quantum chemistry techniques, and performed several exciting applications to materials design and discovery, to make the impact of the infrastructure and methodological work more clearly visible.

1.1 Modular software for atomistic ML

An important milestone from the point of view of the software infrastructure has been the release on PyPI of an alpha version of Metatensor[1], a library that provides a custom sparse array format containing all the required metadata to exchange data between different parts of the ecosystem. Metatensor is compatible with Pytorch's torchscript framework, making it possible to train models in Python and export them in a format that can be loaded from compiled simulation engines such as LAMMPS.
Metatensor facilitates interfacing the various components of the M-stack ecosystem, such as Rascaline[2], that computes representations of atomic structures, and the packages in Q-stack[3], that are geared towards the calculation and manipulation of quantum mechanical quantities, such as different types of scalar fields based on the electron density.

Work is also underway to provide efficient, multi-language and multi-platform libraries to accelerate the calculation of some of the key ingredients of an atomistic ML model. Sphericart[4] provides an efficient implementation of the evaluation of spherical harmonics [1] for both CPU and GPUs, with Python, Pytorch and Jax bindings, that has already received much interest from the community, with the group of Christoph Ortner having contributed a Julia implementation.
The M-stack software ecosystem also includes tools dedicated to structural data manipulation and visualization. For instance, cell2mol[5] [2] provides a platform to automate and streamline calculations for molecular systems, that has already been used to generate several datasets including a curated database[6] of ground-state transition metals complexes and FORMED[7], a dataset containing excited-state properties for 100'000 organic molecules from the CSD [3]. The chemiscope[8] viewer has been extended to include new features such as the visualization of shapes and atomic coloring. To enhance the visibility of these developments, webapps have been deployed on the Materials Cloud, such as an online version of cell2mol[9]. An online calculator to provide access to a SA-GPR (Symmetry-Adapted Gaussian Process Regression) [4] and neural-network frameworks for the prediction of the electron density is also under development (Fig. 1) and will be distributed in early 2024.

1.2 Methodological and algorithmic advances

Following on previous work revealing the limitations of some of the most popular descriptors for atomistic ML [5, 6], we have been able to introduce a set of provably-complete descriptors, based on the definition of low-body-order rotational invariants that correspond to an ensemble of local coordinate systems [7]. A simi-

[1] https://github.com/lab-cosmo/metatensor
[2] https://github.com/Luthaf/rascaline
[3] https://github.com/lcmd-epfl/Q-stack
[4] https://github.com/lab-cosmo/sphericart
[5] https://github.com/lcmd-epfl/cell2mol
[6] https://doi.org/10.24435/materialscloud:zx-t2
[7] https://doi.org/10.24435/materialscloud:aa-2w
[8] https://chemiscope.org/
[9] https://cell2mol.matcloud.xyz/

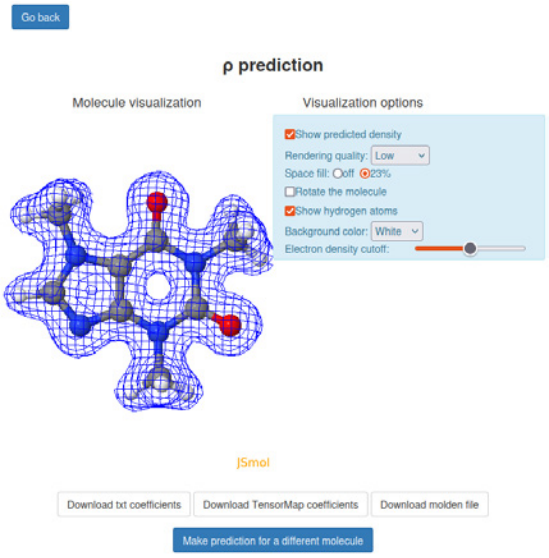


Figure 1: *Screenshot of the predicted electron density for a caffeine molecule on the Materials Cloud.*

lar idea has been developed into the Equivariant Coordinate System Ensemble framework, that allows to incorporate rotational equivariance on top of models that are not equivariant, and that therefore benefit of a larger design space. This has been exploited to develop a point edge transformer (PET) model [8] that achieves state-of-the-art accuracy on several benchmark datasets.

Another important goal in the proposal concerns improvements in uncertainty quantification (UQ) algorithms. Research in the Zdeborová group focused initially on comparing various calibration methods for binary classification in a mathematically tractable high-dimensional model for over-parametrized neural networks. In [9], frequentist and Bayesian inference were compared in terms of UQ, showing that in a model setting based on random-forest features, frequentist methods can be as calibrated as Bayesian methods, when they are used in conjunction with Temperature Scaling, a popular post-training calibration algorithm. A variant of temperature scaling dubbed Expectation Consistency was developed to calibrate the output of neural networks in multi-classification problems [10]. Expectation Consistency outperforms temperature scaling on image classification tasks with different neural network architectures, especially when the test data is corrupted. These ideas (that are implemented in open-source code available online[10]) will be extended to analyze other UQ methods, and applied to atomistic ML.

A major thrust in our methodological effort involves the combination of ML with electronic structure theory. In this respect, there are three main ongoing developments we want to highlight.

(1) The Corminboeuf group has continued with its efforts to design molecular representations that go beyond the description of atomic positions and explicitly include information about the charge and spin of a system. This resulted in a new family of representations: the SPectrum of Approximated Hamiltonian Matrices (SPA$^{\mathrm{H}}$M). The global eigenvalue-based descriptor (ε-SPA$^{\mathrm{H}}$M) [11] is complemented with two local density-matrix-based variants: SPA$^{\mathrm{H}}$M (a) and SPA$^{\mathrm{H}}$M (b). Both encode the information about the electron density of the system using an inexpensive one-electron initial guess [27]. SPA$^{\mathrm{H}}$M (a) results in feature vectors expanded in terms of atoms, and SPA$^{\mathrm{H}}$M (b) localizes the electron density between pairs of atoms, thus affording a description of bonds. These local representations have shown excellent predictive power on local atomic properties (atomic charges, spin densities, and isotropic magnetic shielding) for neutral and charged species of the benchmark database M7 [28] and in a more challenging database of azoheteroarene-based dyes [12]. In particular, SPA$^{\mathrm{H}}$M (b) captures the changes in electron delocalization typically observed in extended π-conjugated systems for both ground and excited states [13]. The performance of both representations is being evaluated against more challenging systems, namely transition metal complexes and chemical reactions [14]. The necessary code and data to generate all SPA$^{\mathrm{H}}$M representations is available online[11].

(2) The Ceriotti group has focused on demonstrating the integration of quantum-mechanical calculations with a predictive ML workflow. By building a symmetry-adapted ML model trained to predict the minimal-basis, single-particle electronic Hamiltonian, and using it as an intermediate layer for predicting a range of target properties such as compute the molecular orbital (MO) energies and Löwdin charges, they demonstrated exceptional transferability to different systems and properties [15]. In particular, they could show that training on a small dataset composed of a few hundred configurations of seven small hydrocarbon molecules allowed making accurate predictions for molecules as large as β-carotene, and to extend the predictions to complex observables such as vibronic

[10] https:/github.com/spoc-group

[11] github.com/lcmd-epfl/SPAHM-RHO

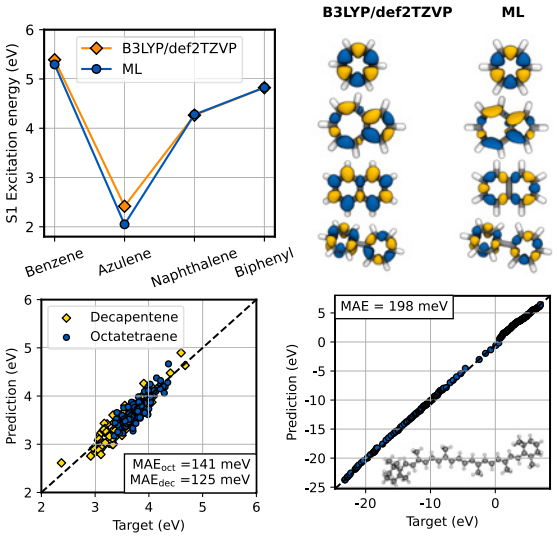


Figure 2: *Extrapolative predictions from an indirect Hamiltonian learning framework. A model trained on a few distorted configurations of seven small hydrocarbons can make accurate predictions of the excitations of some aromatic compounds, long-chain polyenes, and a molecule as complex as β-carotene.*

spectra (Fig. 2).

(3) The Carleo group has worked on incorporating ideas from the ML representation of atomic structures into the many-body description of the electronic structure in molecular as well as extended systems. The primary focus has been the combination of variational Monte Carlo (VMC) with machine-learning techniques, in particular neural networks, to parameterize the many-body wavefunction of the molecular Hamiltonian in the Born-Oppenheimer approximation. Besides technical difficulties such as ensuring the correct quantum statistics, these efforts include the development of expressive features to reduce the learning complexity and therefore computational cost. To this end, in collaboration with the Ceriotti group, many-body atomic descriptors (SOAP and higher-order density-correlation terms), which are traditionally used in the context of energy-surface learning, have been adapted to the description of fermionic degrees of freedom. The systematic dependence of density-correlation features on the correlation order, and on the size of the discrete spherical harmonics/radial functions basis provide more interpretable results as well as fewer variational parameters to optimize. Early experiments on small model systems such as H_2 suggest an improvement upon vanilla Hartree-Fock benchmarks. NetKet, the software used to run the simulations is developed in the Carleo group and can be found online[12].

1.3 Applications and materials design

In order to showcase the algorithms and software developed in this Pillar, we are also actively pursuing more applied projects, targeting materials characterization and design. We want to highlight in particular efforts in the Emsley group to perform structure determination combining NMR measurements and ML predictions. Based on the previously developed model of chemical shifts for molecular solids ShiftML [16], which was recently updated to improve generalization and accuracy [17], a method to directly predict the local three-dimensional environment around atoms in a molecular solid was developed. This makes use of the large-scale computation of chemical shifts in over 300'000 experimental crystal structures using ShiftML2 as previously reported [18]. By comparing the experimental shift associated to a given atomic site with all shifts predicted for similar chemical groups, a chemical shift-dependent three-dimensional interaction map can be generated, which is a first step towards direct prediction of structure from NMR experiments (Fig. 3A) [19]. A general method to determine the structure of amorphous molecular solids at the atomic level was also developed. This involves the large-scale computation of chemical shifts for large ensembles of MD snapshots using ShiftML2, followed by comparison between the experimental chemical shift distributions and the shifts obtained for each molecular environment in the snapshots. By comparing the NMR-selected ensemble comprising molecular environments in best agreement with the NMR experiment to the complete MD ensemble, promoted interactions in the NMR ensemble can be identified (Fig. 3B). This provided the first atomic-level structure of an amorphous molecular solid [20].

We have also been able to extend many of our ongoing investigations of various classes of materials, including ferroelectrics (with a large-scale sampling [21] of polarization fluctuations in $BaTiO_3$, building on a previous collaboration with the Marzari group [22] funded by Samsung), high-entropy alloys (with an extension to surfaces and surface segregation [23] of a breakthrough potential that allows studying arbitrary combinations of 25 transition metals [24], supported by an industrial grant with BASF), precipitation in Al-6xxx alloys [25] (continuing a long-running collaboration be-

[12] github.com/netket/netket

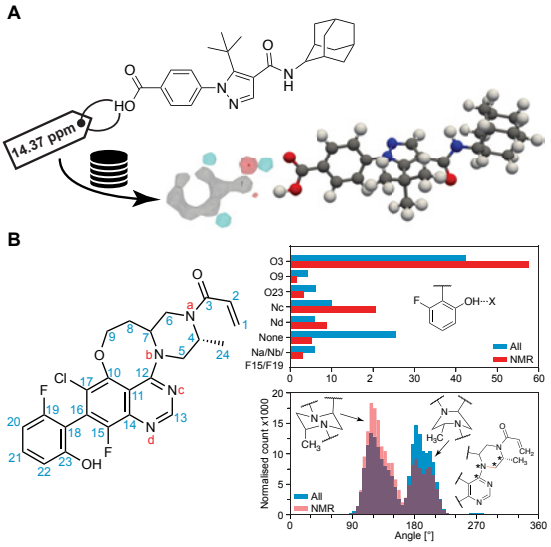


Figure 3: *A. Chemical shift-dependent interaction map around the carboxylic acid proton of AZD8329 constructed using the experimental chemical shift of the crystalline form 1. The interaction map correctly predicts the carboxylic acid dimer present in the crystal structure. B. The structure of the amorphous form of the drug AZD4625 (left) is determined by comparing predicted chemical shifts from MD snapshots to experiments. In comparison to the whole MD ensemble (blue), the ensemble selected based on NMR (red) clearly promotes hydrogen bonding to the enone oxygen and aromatic nitrogens, as well as the chair conformation of the diazinane ring.*

tween the Ceriotti and Curtin groups) and transport in lithium thiophosphate [26].

2 Contribution to overall goals and initial proposal

The focus on the development and release of a high-quality, well-documented and cohesive software infrastructure is perfectly in line with the goals of usability and visibility set forth for the third phase of the NCCR. The parallel efforts to advance our understanding of atomic-scale ML, and the applications to relevant materials-science problems, support and motivate these efforts. The implementation of interactive apps on the Materials Cloud platform showcase the integration of Pillar 2 efforts within the broader scope of MARVEL.

3 Collaborative and interdisciplinary components

This second year has seen the first results from the involvement of partner laboratories, as well as the ongoing joint effort by the Corminboeuf and Ceriotti groups to unify our ML infrastructure. Collaborative efforts with Pillar 1 [25], with industrial partners (BASF and Samsung), as well as with research labs outside MARVEL (e.g., the collaboration with Benedetta Mennucci on ML for electronic excitations [15]) underscore the commitment of the member labs to collaborative research efforts.

MARVEL publications

List of publications either resulting directly from the NCCR (marked with a red hexagon) or with minor contributions from the NCCR.

- [1] F. Bigi, G. Fraux, N. J. Browning, and M. Ceriotti, *Fast evaluation of spherical harmonics with sphericart*, The Journal of Chemical Physics **159**, 064802 (2023).
- [2] S. Vela, R. Laplaza, Y. Cho, and C. Corminboeuf, *cell2mol: encoding chemistry to interpret crystallographic data*, npj Computational Materials **8**, 188 (2022).
- [3] J. T. Blaskovits, R. Laplaza, S. Vela, and C. Corminboeuf, *Data-Driven Discovery of Organic Electronic Materials Enabled by Hybrid Top-Down/Bottom-Up Design*, Advanced Materials **2023**, 2305602 (2023).
- [4] A. Grisafi, A. Fabrizio, B. Meyer, D. M. Wilkins, C. Corminboeuf, and M. Ceriotti, *Transferable Machine-Learning Model of the Electron Density*, ACS Central Science **5**, 57 (2019).
- [5] S. N. Pozdnyakov, L. Zhang, C. Ortner, G. Csányi, and M. Ceriotti, *Local invertibility and sensitivity of atomic structure-feature mappings*, Open Research Europe **1**, 126 (2021).
- [6] S. N. Pozdnyakov and M. Ceriotti, *Incompleteness of Graph Neural Networks for Points Clouds in Three Dimensions*, Machine Learning: Science and Technology **3**, 045020 (2022).
- [7] J. Nigam, S. N. Pozdnyakov, K. K. Huguenin-Dumittan, and M. Ceriotti, *Completeness of Atomic Structure Representations*, arXiv:2302.14770 (2023).
- [8] S. N. Pozdnyakov and M. Ceriotti, *Smooth, exact rotational symmetrization for deep learning on point clouds*, arXiv:2305.19302 (2023).
- [9] L. Clarté, B. Loureiro, F. Krzakala, and L. Zdeborová, *On double-descent in uncertainty quantification in overparametrized models*, in *Proceedings of The 26th International Conference on Artificial Intelligence and Statistics*, F. Ruiz, J. Dy, and J.-W. van de Meent, eds. (PMLR, 2023), vol. 206 of *Proceedings of Machine Learning Research*, pp. 7089–7125.
- [10] L. Clarté, B. Loureiro, F. Krzakala, and L. Zdeborová, *Expectation consistency for calibration of neural networks*, in *Proceedings of the Thirty-Ninth Conference on Uncertainty in Artificial Intelligence*, R. J. Evans and I. Shpitser, eds. (PMLR, 2023), vol. 216 of *Proceedings of Machine Learning Research*, pp. 443–453.
- [11] A. Fabrizio, K. R. Briling, and C. Corminboeuf, *SPA^{H}M: the spectrum of approximated Hamiltonian matrices representations*, Digital Discovery **1**, 286 (2022).
- [12] S. Vela, A. Fabrizio, K. R. Briling, and C. Corminboeuf, *Learning the Exciton Properties of Azo-dyes*, The Journal of Physical Chemistry Letters **12**, 5957 (2021).
- [13] K. R. Briling, Y. Calvino Alonso, A. Fabrizio, and C. Corminboeuf, *SPA^{H}M(a,b): Encoding the Density Information from Guess Hamiltonian in Quantum Machine Learning Representations*, Journal of Chemical Theory and Computation (2024), doi:10.1021/acs.jctc.3c01040.

[14] P. van Gerwen, K. R. Briling, Y. Calvino Alonso, M. Franke, and C. Corminboeuf, *Benchmarking machine-readable vectors of chemical re- actions on computed activation barriers*, ChemRxiv. Preprint. (2023), doi:10.26434/chemrxiv-2023-0hgbc.

[15] E. Cignoni, D. Suman, J. Nigam, L. Cupellini, B. Mennucci, and M. Ceriotti, *Electronic excited states from physically-constrained machine learning*, arXiv:2311.00844 (2023).

[16] F. M. Paruzzo, A. Hofstetter, F. Musil, S. De, M. Ceriotti, and L. Emsley, *Chemical shifts in molecular solids by machine learning*, Nature Communications **9**, 4501 (2018).

[17] M. Cordova, E. A. Engel, A. Stefaniuk, F. Paruzzo, A. Hofstetter, M. Ceriotti, and L. Emsley, *A Machine Learning Model of Chemical Shifts for Chemically and Structurally Diverse Molecular Solids*, The Journal of Physical Chemistry C **126**, 16710 (2022).

[18] M. Cordova, M. Balodis, B. Simões de Almeida, M. Ceriotti, and L. Emsley, *Bayesian probabilistic assignment of chemical shifts in organic solids*, Science Advances **7**, eabk2341 (2021).

[19] M. Cordova and L. Emsley, *Chemical Shift-Dependent Interaction Maps in Molecular Solids*, Journal of the American Chemical Society **145**, 16109 (2023).

[20] M. Cordova, P. Moutzouri, S. O. N. Lill, A. Cousen, M. Kearns, S. T. Norberg, A. S. Ankarberg, J. McCabe, A. C. Pinon, S. Schantz, and L. Emsley, *Atomic-level structure determination of amorphous molecular solids by NMR*, Nature Communications **14**, 5138 (2023).

[21] L. Gigli, A. Goscinski, M. Ceriotti, and G. A. Tribello, *Modeling the ferroelectric phase transition in barium titanate with DFT accuracy and converged sampling*, arXiv:2310.12579 (2023).

[22] L. Gigli, M. Veit, M. Kotiuga, G. Pizzi, N. Marzari, and M. Ceriotti, *Thermodynamics and dielectric response of $BaTiO_3$ by data-driven modeling*, npj Computational Materials **8**, 209 (2022).

[23] A. Mazitov, M. A. Springer, N. Lopanitsyna, G. Fraux, S. De, and M. Ceriotti, *Surface segregation in high-entropy alloys from alchemical machine learning*, arXiv:2310.07604 (2023).

[24] N. Lopanitsyna, G. Fraux, M. A. Springer, S. De, and M. Ceriotti, *Modeling high-entropy transition metal alloys with alchemical compression*, Physical Review Materials **7**, 045802 (2023).

[25] A. C. P. Jain, M. Ceriotti, and W. A. Curtin, *Natural aging and vacancy trapping in Al-6xxx*, Journal of Materials Research **38**, 5171 (2023).

[26] L. Gigli, D. Tisi, F. Grasselli, and M. Ceriotti, *Mechanism of charge transport in lithium thiophosphate*, arXiv:2310.15679 (2023).

Other references

[27] D. N. Laikov and K. R. Briling, *Atomic effective potentials for starting molecular electronic structure calculations*, Theoretical Chemistry Accounts **139**, 17 (2020).

[28] M. Rupp, A. Tkatchenko, K.-R. Müller, and O. A. von Lilienfeld, *Fast and accurate modeling of molecular atomization energies with machine learning*, Physical Review Letters **108**, 058301 (2012).

List of year 10 publications related to Pillar 2

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).

⬣○ K. R. Briling, Y. Calvino Alonso, A. Fabrizio, and C. Corminboeuf

$SPA^{H}M(a,b)$: Encoding the Density Information from Guess Hamiltonian in Quantum Machine Learning Representations

Journal of Chemical Theory and Computation (2024), doi:10.1021/acs.jctc.3c01040.

Group(s): Corminboeuf / Project(s): P2

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:1g-w5

⬣○ J. T. Blaskovits, R. Laplaza, S. Vela, and C. Corminboeuf

Data-Driven Discovery of Organic Electronic Materials Enabled by Hybrid Top-Down/Bottom-Up Design

Advanced Materials **2023**, 2305602 (2023).

Group(s): Corminboeuf / Project(s): P2

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:aa-2w

⬣○ F. Bigi, G. Fraux, N. J. Browning, and M. Ceriotti

Fast evaluation of spherical harmonics with sphericart

The Journal of Chemical Physics **159**, 064802 (2023).

Group(s): Ceriotti / Project(s): P2

Links to article: Journal / Open access

Related datasets: github.com/lab-cosmo/sphericart

⬣○ L. Clarté, B. Loureiro, F. Krzakala, and L. Zdeborová

Expectation consistency for calibration of neural networks

in *Proceedings of the Thirty-Ninth Conference on Uncertainty in Artificial Intelligence*, R. J. Evans and I. Shpitser, eds. (PMLR, 2023), vol. 216 of *Proceedings of Machine Learning Research*, pp. 443–453.

Group(s): Zdeborova / Project(s): P2

Links to article: Journal / Open access

Related datasets: doi.org/10.24435/materialscloud:ws-p3

N. Lopanitsyna, G. Fraux, M. A. Springer, S. De, and M. Ceriotti
Modeling high-entropy transition metal alloys with alchemical compression
Physical Review Materials **7**, 045802 (2023).
Group(s): Ceriotti / Project(s): P2
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:73-yn

L. Clarté, B. Loureiro, F. Krzakala, and L. Zdeborová
On double-descent in uncertainty quantification in overparametrized models
in *Proceedings of The 26th International Conference on Artificial Intelligence and Statistics*, F. Ruiz, J. Dy, and J.-W. van de Meent, eds. (PMLR, 2023), vol. 206 of *Proceedings of Machine Learning Research*, pp. 7089–7125.
Group(s): Zdeborova / Project(s): P2
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:zb-71

R. K. Cersonsky, M. Pakhnova, E. A. Engel, and M. Ceriotti
A data-driven interpretation of the stability of organic molecular crystals
Chemical Science **14**, 1272 (2023).
Group(s): Ceriotti / Project(s): P2, DD1
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:71-21

A. C. P. Jain, M. Ceriotti, and W. A. Curtin
Natural aging and vacancy trapping in Al-6xxx
Journal of Materials Research **38**, 5171 (2023).
Group(s): Ceriotti, Curtin / Project(s): P1, P2
Links to article: Journal / Open access
Related datasets: not applicable

G. Pescia, J. Nys, J. Kim, A. Lovato, and G. Carleo
Message-Passing Neural Quantum States for the Homogeneous Electron Gas
arXiv:2305.07240 (2023).
Group(s): Carleo / Project(s): P2
Links to article: Journal / Open access
Related datasets: not applicable

A. Mazitov, M. A. Springer, N. Lopanitsyna, G. Fraux, S. De, and M. Ceriotti
Surface segregation in high-entropy alloys from alchemical machine learning
arXiv:2310.07604 (2023).
Group(s): Ceriotti / Project(s): P2
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:ps-20

S. N. Pozdnyakov and M. Ceriotti
Smooth, exact rotational symmetrization for deep learning on point clouds
arXiv:2305.19302 (2023).
Group(s): Ceriotti / Project(s): P2
Links to article: Journal / Open access
Related datasets: not applicable

L. Gigli, D. Tisi, F. Grasselli, and M. Ceriotti
Mechanism of charge transport in lithium thiophosphate
arXiv:2310.15679 (2023).
Group(s): Ceriotti / Project(s): P2
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:g2-fp

E. Cignoni, D. Suman, J. Nigam, L. Cupellini, B. Mennucci, and M. Ceriotti
Electronic excited states from physically-constrained machine learning
arXiv:2311.00844 (2023).
Group(s): Ceriotti / Project(s): P2
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:5s-gm

J. Nigam, S. N. Pozdnyakov, K. K. Huguenin-Dumittan, and M. Ceriotti
Completeness of Atomic Structure Representations
arXiv:2302.14770 (2023).
Group(s): Ceriotti / Project(s): P2
Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.8003293

L. Gigli, A. Goscinski, M. Ceriotti, and G. A. Tribello
Modeling the ferroelectric phase transition in barium titanate with DFT accuracy and converged sampling
arXiv:2310.12579 (2023).
Group(s): Ceriotti / Project(s): P2
Links to article: Journal / Open access
Related datasets: not applicable

P. van Gerwen, K. R. Briling, Y. Calvino Alonso, M. Franke, and C. Corminboeuf
Benchmarking machine-readable vectors of chemical re- actions on computed activation barriers
ChemRxiv. Preprint. (2023), doi:10.26434/chemrxiv-2023-0hgbc.
Group(s): Corminboeuf / Project(s): P2
Links to article: Journal / Open access
Related datasets: not applicable

Pillar 3 — Digital Infrastructure of Open Simulations and Data

Project leaders: Giovanni Pizzi (EPFL), **Joost VandeVondele** (CSCS)

Partners: Sara Bonella (EPFL), **Michael Herbst** (EPFL)

1 Progress of the different efforts

1.1 AiiDA and high-throughput workflows for materials discovery and characterization

In year 10, three new versions of AiiDA were released (2.3, 2.4, 2.5). Recent developments focused on making AiiDA easier for users, including automated environment setup[1] and lightweight profiles not requiring configuration of any system service. We also strengthened the support for the new Alps infrastructure, with a proof-of-concept implementation of connections via the FirecREST API and native support for containerized codes, including the SARUS engine.

To streamline interaction and support within the AiiDA community, we transitioned from a mailing list to a new platform on Discourse[2], where 340+ posts have already appeared since July 2023. As a Google Summer of Code project, the AiiDA plugin registry[3] was redesigned, making it easier than ever to search and inspect existing plugins. The registry now includes 92 plugin packages with over 160 workflows, developed for dozens of popular codes in the materials science community, including a set of new workflows that we developed for automated Wannierization [1, 2]. These have been combined with the phonon workflows presented in the year 9 report to integrate AiiDA with the EPW code[4], which enables automated calculation of the electron-phonon interactions. A screening of the MC3D database for novel superconductors is ongoing using these exciting new workflows.

The common workflow interface discussed in the year 9 report was used for a large-scale verification study published on *Nature Reviews Physics* [3]. The work includes a high-quality all-electron reference dataset (obtained with the two codes FLEUR and WIEN2k), then used to verify 9 other pseudopotential codes (Fig. 1) and improve the respective pseudopotential libraries. Notably, our AiiDAlab SSSP toolkit (see year 9 report) was used to produce two new releases of SSSP (v1.2 and v1.3), improving existing pseudopotentials and extending them to include actinides.

Similar to the LUMI-C "hero run" discussed in the year 9 report, we could obtain a dedicated slot on the new LUMI-G partition (2'978 nodes with 4 AMD MI250x GPUs + one 64-core AMD EPYC "Trento" CPU). During a 9-hour time window, AiiDA was used to run 22'353 SIRIUS-enabled QUANTUM ESPRESSO calculations (Fig. 2a). Running with SIRIUS was crucial because (i) it enabled running QUANTUM ESPRESSO on the LUMI-G AMD architecture, and (ii) it provided the new robust direct minimization technique (see year 9 report). Using a multi-step approach, we successfully determined the ground-state geometry of 2'978 structures that failed with regular QUANTUM ESPRESSO, reaching a noteworthy success rate of 95% for the new SIRIUS-enabled workflow. We note that the AiiDA submission rate was so high to overwhelm the SLURM scheduler afrew a few hours (Fig. 2a). To overcome this limitation for high-throughput runs, we developed a new scheduler plugin interfacing with HyperQueue[5] (Fig. 2b), a "meta-scheduler" that

[1] https://github.com/aiidateam/aiida-project
[2] https://aiida.discourse.group/
[3] https://aiidateam.github.io/aiida-registry/
[4] https://epw-code.org/
[5] https://github.com/aiidateam/aiida-hyperqueue

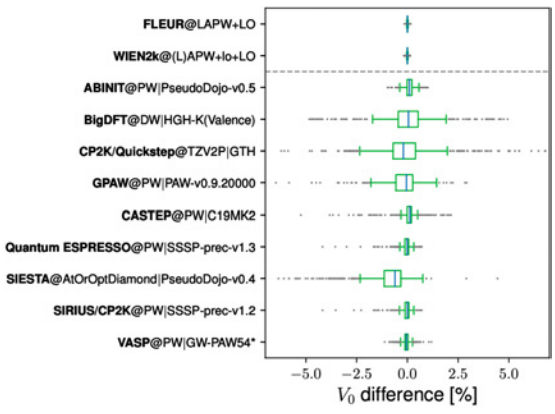


Figure 1: *Box-and-whisker plots comparing the volume discrepancy of 11 codes involved in [3], with respect to the all-electron reference dataset.*

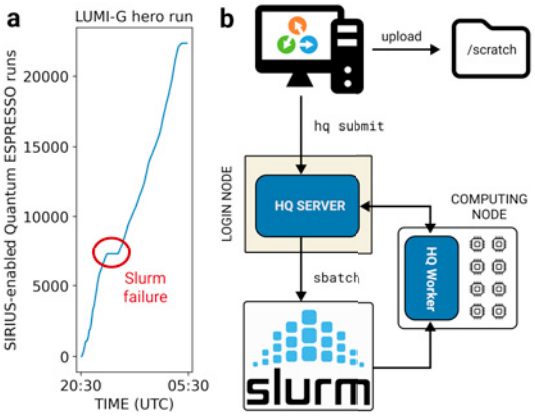


Figure 2: *(a) Total number of completed SIRIUS-enabled* QUANTUM ESPRESSO *runs during the LUMI-G hero run. (b) Flow chart explaining how AiiDA uses the HyperQueue (HQ) meta-scheduler to avoid overloading the scheduler.*

batches multiple AiiDA submissions in a single scheduler job, enabling higher submission rates and more efficient use of the scheduler queue.

1.2 Materials Cloud

Materials Cloud remains widely used by the materials science community, with over 160K unique visits between January and October 2023 (a 20% increase with respect to the same period in 2022). Multiple *Discover* sections have received updates. Notably, the Materials Cloud 3D crystals database (MC3D)[6] was reimplemented with the React framework and now includes various improvements, such as advanced filtering and searching (Fig. 3). Moreover, a new *Discover* section was added with the curated data associated to the DFT verification[7] paper discussed earlier [3].

The *Work* section now contains OSSCAR (Open Software Services for Classrooms and Research)[8], a platform hosting software and tools geared towards education and research. The *Learn* section has expanded to include 259 recordings of lectures and tutorials, and the transition to Lhumos is progressing steadily (see next section).

The *Archive*, our open access and moderated research data repository, continues to grow (172 new records since January 2023 and a total of 922 records, as of November 13, 2023). The development of a new version of the *Archive* using InvenioRDM[9] is ongoing, with the new version planned to go in

[6] https://materialscloud.org/mc3d
[7] https://materialscloud.org/acwf-verification
[8] https://osscar.org
[9] https://inveniordm.docs.cern.ch/

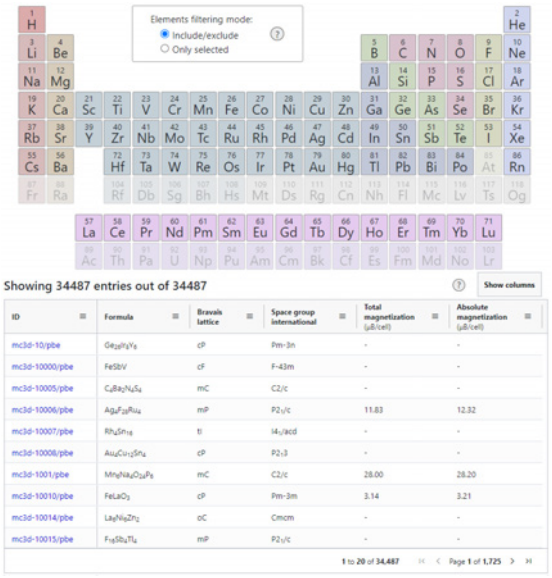


Figure 3: *Search interface of the new MC3D Discover section, allowing for advanced filtering and data display.*

production upon CERN's release of InvenioRDM LTS v12, scheduled for spring 2024. The new version will bring several new features and a more user-friendly interface, including drag-and-drop file upload, parallel upload of several files, support of fast addition of authors/affiliations via a dropdown and/or via their ORCID ID, generation of secret links for secure access to the record by collaborators, and extensive REST APIs supporting all repository operations. Finally, the *Archive*-OPTIMADE service was developed. By simply uploading crystal structures in an *Archive* entry (together with a very simple configuration file), we generate a custom OPTIMADE API[10] to serve the structures in a standard way, allowing researchers to access them via any OPTIMADE-compliant tool. A prototype demo server is already online[11].

1.3 Lhumos

Lhumos is the next generation platform for educational material, designed to replace Materials Cloud *Learn*. In year 10, significant developments enabled the deployment of an alpha version[12] (Fig. 4). Moreover, Lhumos has been populated with training material; migration of all Materials Cloud *Learn* content will be completed in early 2024. Testing within a broad user pool is ongoing; feedback on issues and user experience will be collected and inte-

[10] https://www.optimade.org/
[11] https://dev-optimade.materialscloud.org/
[12] https://alpha.lhumos.org

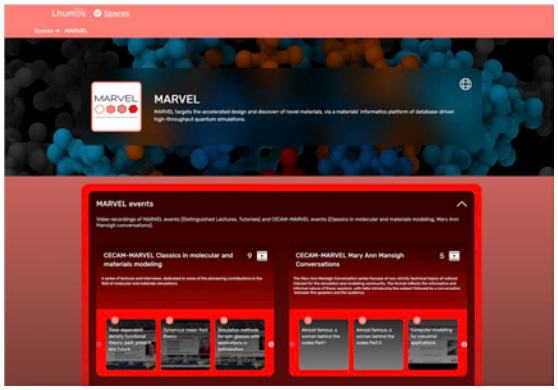


Figure 4: *Alpha Lhumos platform.*

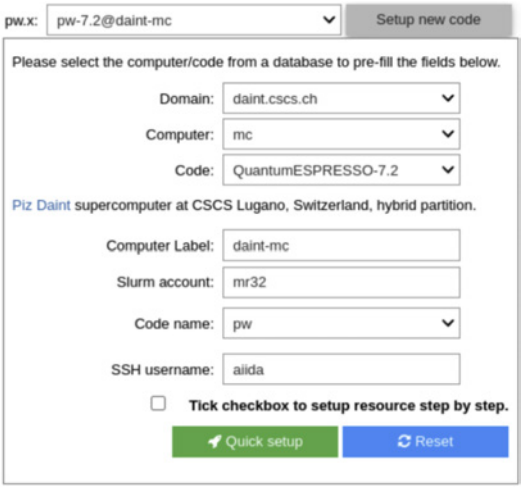


Figure 5: *Setting up a* `pw.x` *code on a CSCS machine via the redesigned AiiDAlab resource setup widget.*

grated in the beta release, foreseen for Q2 2024. The EU Centre of Excellence MultiXscale[13] will open a new space on Lhumos in early 2024, and discussions have been initiated with two more projects, BioNT[14] and Dome 4.0[15] for access to the platform.

1.4 AiiDAlab and Quantum Mobile

In year 10 there have been two releases of the Quantum Mobile virtual machine. The latest version of the AiiDAlab QUANTUM ESPRESSO (QE) app (v23.10.0) contains several notable features, including a new image that streamlines the initiation and execution of QUANTUM ESPRESSO calculations without additional setup. We also implemented a robust test suite covering ∼80% of the code, ensuring reliability and stability of the application. A newly designed widget makes the setup of new resources (remote computers and code executables) very easy (Fig. 5). The QE app now has a plugin design, paving the way to adding custom interfaces to compute advanced properties (such as XAS and XPS spectroscopies, Raman and IR phonon spectra, or muon spectroscopy, see Pillar 4).
New AiiDAlab applications have been registered, such as the Aurora app[16], an Empa-EPFL-PSI collaboration targeting autonomous battery optimization, where AiiDA-tracked cycling experiments of robot-assembled coin cells can be launched and monitored from the app [4]. The In Silico Photochemistry group of Bristol University contributes now actively to the development of AiiDAlab and released the ATMOSPEC app[17], encapsulating an *ab initio* workflow for UV/VIS spectroscopy of organic molecules. Our recent endeavors also include the deployment of AiiDAlab for the NEP project[18] on CSCS, as well as a new internal deployment for experimentalists at PSI (in collaboration with Pillar 4), demonstrating a commitment to fostering collaborative research environments and facilitating seamless workflows for researchers.

1.5 SIRIUS, and MaZe integration

We successfully implemented LDA+U+V for SIRIUS, expanded `nlcglib`[19] to accommodate Hubbard functionality, and implemented a magnetism-constrained Hubbard approach for finding the correct magnetic ground state. The `nlcglib` package now also supports distributed wavefunctions and GPUDirect RDMA. Linear wavefunction extrapolation has been added to C++ SIRIUS improving MD support of `q-e-sirius`. The beta-projector code in SIRIUS has been refactored to better accommodate the needs of the ultrasoft preconditioning required in `nlcglib`.
Collaborative work between the Bonella group (EPFL) and CSCS led to the implementation via the Python binders for the SIRIUS library of a suite of first principles molecular dynamics algorithms, including Born-Oppenheimer, Car-Parrinello, Extended Lagrangian Method, and Kolafa Algorithm. These are the first demonstrators of the use of SIRIUS as a driver for simulations of time-dependent properties of materials, and pave the way for combining the Mass Zero (MaZe) Constrained Dynamics with SIRIUS.

[13] https://www.multixscale.eu/
[14] https://biont-training.eu/
[15] https://dome40.eu/
[16] https://github.com/epfl-theos/aiidalab-aurora
[17] https://github.com/ispg-group/aiidalab-ispg
[18] https://nffa.eu/news/project-updates/pilot-nep/
[19] https://github.com/simonpintarelli/nlcglib

1.6 DFTK: An interdisciplinary DFT code tailored towards mathematical research

In year 10 the team of Michael Herbst (EPFL) joined, adding the density-functional toolkit (DFTK)[20] to the MARVEL software portfolio. DFTK is being integrated with AiiDA and we released a DFTK plugin[21], currently being used for a full-scale verification using the dataset from [3]. Initial results show that DFTK is in very good agreement with standard codes, with a few outliers that we are now investigating, probably because of details of the pseudopotential handling. In the upcoming years, the goal is to expand the verification beyond equations of state and to employ the plugin to verify a recently developed technique for estimating the error due to insufficient plane wave cutoffs [5] on a broader range of systems.

2 Contribution to overall goals and initial proposal

The exascale readiness of SIRIUS and AiiDA has been further validated on exascale infrastructures through the LUMI-G hero run, benefitting from enhanced robustness due to the direct minimization methods within SIRIUS. This is complemented by a high-impact verification process that utilizes common workflows to produce refined parameters, crucial for automated workflows. Integration between MaZe and SIRIUS has also been achieved. Moreover, the Materials Cloud *Archive* continues to grow, securing its position as a key repository for materials science data. Additionally, the Lhumos platform has seen its inaugural deployment.

3 Collaborative and interdisciplinary components

There are several ongoing European collaborations, including with TIER-0 HPC centers, Battery2030+'s BIG-MAP, and several H2020 projects like MaX and TREX Centres of excellence. The new ORD-R Establish initiative "PREMISE", led by Giovanni Pizzi and supported by the ETH Domain, has adopted AiiDA as the main workflow engine for simulations and robotic experiments. In partnership with H2020 BIG-MAP, a successful autonomous loop for battery experiments controlled by AiiDA through an AiIDAlab GUI has been demonstrated [4]. In addition, tight collaborations are ongoing with the SNSF project FISH4DIET, led by Giovanni Pizzi, focusing on high-throughput discovery of materials with exceptional Fermi surface topologies, where a workflow has been set up to automatically obtain a Wannier-function representation of any material and then predict Shubnikov-de Haas oscillation frequencies.

The common-workflows verification project is a massive collaboration with over 45 partners worldwide, including several key players in the *ab initio* community. This consortium will continue to work together on testing the tools we all rely on, where AiiDA will play a central role as the workflow engine. In a combined effort by the AiiDAlab and CSCS teams, we have introduced the MFA CSCS app[22], designed to simplify the setup of CSCS machines under its multi-factor authentication. This cooperative effort aims to streamline processes, making AiiDAlab more accessible and user-friendly for researchers utilizing CSCS resources.

The development and deployment of the Lhumos portal is part of a collaborative effort with CECAM and the EU funded Centre of excellence for computing applications MaX[23]. Uploading of training material from the three centers is part of a broader effort to provide a unique entry point for advanced education in simulation and modeling, with a particular focus on tools for the simulation of materials.

MARVEL publications

List of publications either resulting directly from the NCCR (marked with a red hexagon) or with minor contributions from the NCCR.

- [1] J. Qiao, G. Pizzi, and N. Marzari, *Projectability disentanglement for accurate and automated electronic-structure Hamiltonians*, npj Computational Materials **9**, 208 (2023).
- [2] J. Qiao, G. Pizzi, and N. Marzari, *Automated mixing of maximally localized Wannier functions into target manifolds*, npj Computational Materials **9**, 206 (2023).
- [3] E. Bosoni, L. Beal, M. Bercx, P. Blaha, S. Blügel, J. Bröder, M. Callsen, S. Cottenier, A. Degomme, V. Dikan, K. Eimre, E. Flage-Larsen, M. Fornari, A. Garcia, L. Genovese, M. Giantomassi, S. P. Huber, H. Janssen, G. Kastlunger, M. Krack, G. Kresse, T. D. Kühne, K. Lejaeghere, G. K. H. Madsen, M. Marsman, N. Marzari, G. Michalicek, H. Mirhosseini, T. M. A. Müller, G. Petretto, C. J. Pickard, S. Poncé, G.-M. Rignanese, O. Rubel, T. Ruh, M. Sluydts, D. E. P. Vanpoucke, S. Vijay, M. Wolloch, D. Wortmann, A. V. Yakutovich, J. Yu, A. Zadoks, B. Zhu, and G. Pizzi, *How to verify the precision of density-functional-theory implementations via reproducible and universal workflows*, Nature Reviews Physics **6**, 45 (2024).
- [4] 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*, ChemRxiv. Preprint. (2023), doi:10.26434/chemrxiv-2023-4vs5w.

[20] https://dftk.org
[21] https://github.com/aiidaplugins/aiida-dftk
[22] https://github.com/aiidalab/aiidalab-mfa-cscs
[23] http://www.max-centre.eu/

Other references

[5] E. Cancès, G. Dusson, G. Kemlin, and A. Levitt, *Practical Error Bounds for Properties in Plane-Wave Electronic Structure Calculations*, SIAM Journal on Scientific Computing **44**, B1312 (2022).

List of year 10 publications related to Pillar 3

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).

⬢○ P. Bonfà, I. J. Onuorah, F. Lang, I. Timrov, L. Monacelli, C. Wang, X. Sun, O. Petracic, G. Pizzi, N. Marzari, S. J. Blundell, and R. De Renzi
Magnetostriction-Driven Muon Localization in an Antiferromagnetic Oxide
Physical Review Letters **132**, 046701 (2024).
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:8s-qh

⬢○ E. Bosoni, L. Beal, M. Bercx, P. Blaha, S. Blügel, J. Bröder, M. Callsen, S. Cottenier, A. Degomme, V. Dikan, K. Eimre, E. Flage-Larsen, M. Fornari, A. Garcia, L. Genovese, M. Giantomassi, S. P. Huber, H. Janssen, G. Kastlunger, M. Krack, G. Kresse, T. D. Kühne, K. Lejaeghere, G. K. H. Madsen, M. Marsman, N. Marzari, G. Michalicek, H. Mirhosseini, T. M. A. Müller, G. Petretto, C. J. Pickard, S. Poncé, G.-M. Rignanese, O. Rubel, T. Ruh, M. Sluydts, D. E. P. Vanpoucke, S. Vijay, M. Wolloch, D. Wortmann, A. V. Yakutovich, J. Yu, A. Zadoks, B. Zhu, and G. Pizzi
How to verify the precision of density-functional-theory implementations via reproducible and universal workflows
Nature Reviews Physics **6**, 45 (2024).
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:s4-3h

⬢○ D. Campi, N. Mounet, M. Gibertini, G. Pizzi, and N. Marzari
Expansion of the Materials Cloud 2D Database
ACS Nano **17**, 11268 (2023).
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:36-nd

⬢○ M. Bonacci, J. Qiao, N. Spallanzani, A. Marrazzo, G. Pizzi, E. Molinari, D. Varsano, A. Ferretti, and D. Prezzi
Towards high-throughput many-body perturbation theory: efficient algorithms and automated workflows
npj Computational Materials **9**, 74 (2023).
Group(s): Pizzi / Project(s): P3
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:6w-qh

⬢○ J. Qiao, G. Pizzi, and N. Marzari
Projectability disentanglement for accurate and automated electronic-structure Hamiltonians
npj Computational Materials **9**, 208 (2023).
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:x0-yf

⬢○ J. Qiao, G. Pizzi, and N. Marzari
Automated mixing of maximally localized Wannier functions into target manifolds
npj Computational Materials **9**, 206 (2023).
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:2f-hs

⬢○ 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
ChemRxiv. Preprint. (2023), doi:10.26434/chemrxiv-2023-4vs5w.
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:qh-gt

○ 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
The Wannier-Functions Software Ecosystem for Materials Simulations
arXiv:2312.10769 (2023).
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: not applicable

Pillar 4 Long-term Integration in the Swiss Scientific Landscape

Project leaders: Nicola Marzari (EPFL and PSI), **Christian Rüegg** (PSI), **Carlo Pignedoli** (Empa)

Partners: Ana Akrap (UniFR), Emiliana Fabbri (PSI)

1 Progress of the different efforts

1.1 Computational spectroscopies

a) *X-ray absorption and photoelectron spectroscopies* We implement automated and robust workflows, namely XpsWorkChain and XspectraBaseWorkChain, to compute the core-level spectra, namely X-ray absorption spectroscopy (XAS) and X-ray photoemission spectroscopy (XPS), using AiiDA and QUANTUM ESPRESSO (QE). These workflows utilize core-excited pseudopotentials and offer various options (e.g., full, excited, or half core-hole) for the core hole treatment. The workflows handle the advanced setup for various materials (e.g., crystals, molecules, and other systems with low symmetry), taking care of the identification of symmetry-inequivalent atoms and the supercell generation needed to take into account of the core hole in periodic boundary conditions. We are actively applying these workflows for various systems, aiding experimentalists in spectrum calculation and peak assignment. Our ongoing collaborations include Mounir Mensi from EPFL on XPS in copper oxide, Luca Artiglia from PSI on XPS of Pt nanoparticles, and Mario El Kazzi from PSI on XAS of battery materials (e.g., $LiMn_2O_4$). On the other hand, thanks to the new plugin implementation of the AiiDAlab QEapp in Pillar 3, we can now seamlessly develop and incorporate spectroscopy calculations as plugins within the AiiDAlab platform. Our ongoing effort focuses on integrating these workflows into the AiiDAlab QEapp. This integration aims to provide a user-friendly interface accessible directly through a web browser. It will enable researchers from EPFL, PSI, Empa and other institutions to perform core-level spectra calculations and visualize the results without needing to write any code. Fig. 1 (left) illustrates the XPS AiiDA plugin.

b) *Inelastic neutron scattering spectroscopy* Towards leveraging the data analysis and interpretation capabilities of experimental laboratories at PSI, e.g., the neutron scattering facilities, we are developing workflows to model the magnetic interactions of materials from *ab initio*. We parameterize a generalized Heisenberg Hamiltonian, including the Dzyaloshinskii-Moriya interaction, using the magnetic force theorem [11]. Our approach consists of combining QE, Wannier90, TB2J, and DFWannier codes. We chose this route based on the need for Hubbard corrections, as implemented in QE, that have been shown essential to describe the ground-state properties of magnetic materials. We performed an extensive validation by comparing our results for elemental magnetic materials (e.g., bulk Fe, Ni, and Co) against a full electron DFT code (JuKKR) (Fig. 1, right). The results are very promising, and currently, we are investigating the source of small discrepancies. Meanwhile, we have also researched the topological magnons in Mn_5Ge_3 [1]. In addition, we are working on the implementation of the on-site U and inter-site V Hubbard corrections [2] in the noncollinear framework of time-dependent density-functional theory (TDDFT) including spin-orbit coupling (SOC). This will result in the so-called TDDFT+U+V approach for modeling magnons in complex transition-metal compounds that require the Hubbard corrections. Leveraging the existing TDDFT implementation in QE, known as the TURBOMAGNON code [3], our ongoing efforts focus on the testing and validation of our TDDFT+U implementation. Within the independent particle approximation, the computed TDDFT+U Stoner spectrum demonstrates noteworthy agreement with the reference spectrum derived from a straightforward calculation using the sum over empty states. Simultaneously, we are assessing the accuracy of the implemented response Hubbard potential by comparing it to calculations performed using the Heisenberg model Hamiltonian, using TB2J. Concomitantly, we are actively extending our work to incorporate the $+V$ term, aiming to realize the complete TDDFT+U+V framework.

c) *Muon Spin spectroscopy* Muon spin rotation/resonance (μSR) is among the most effi-

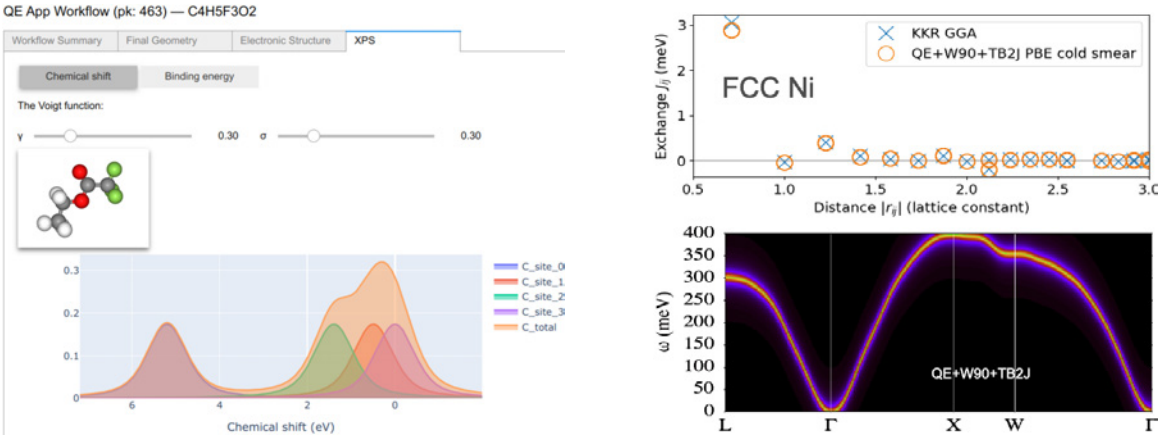


Figure 1: *Left: XPS calculation for the $C_4H_5F_3O_2$ molecule using the AiiDAlab-XPS workflow in the QEapp. Right: Heisenberg exchange parameters of bulk Ni computed using QE+Wannier90+TB2J vs JuKKR, and the resulting spin-wave dispersion of the former method.*

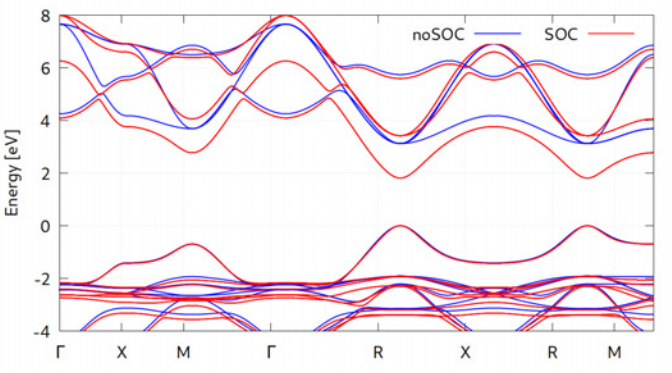
cient techniques used to study several material properties, e.g., magnetism, superconductivity, defects, as well as hydrogen diffusion. We contributed to the development of automated workflows within the AiiDA framework, devoted to characterize the different muon stopping sites in materials from an *ab initio* perspective [12]. This is done in collaboration with Pietro Bonfà and Ifeanyi John Onuorah, both from the University of Parma (Italy). In particular, two AiiDA workflows are developed for such a purpose, called FindMuonWorkchain and MusconvWorkchain and delivered within the `aiida-muon` and the `aiida-musconv` codes. These workchains use QE and other post processing codes in order to relax a given supercell containing the muon candidate and compute, if any, the magnetic field at the muon site. An intuitive graphical user interface is also provided in the AiiDAlab framework, thanks to the above mentioned plugin implementation of the AiiDAlab QEapp. This opens the possibility to perform μSR simulations on a daily routine alongside experimental measurements at PSI and will promote wider adoption of *ab initio* methods by the μSR community.

d) *Photoemission spectroscopy* Koopmans spectral functionals provide a theoretical framework that allows to obtain reliable charged excitations (as revealed, e.g., in photoemission and angle-resolved photoemission spectroscopies) of molecules and materials within a functional approach. The framework, and its deployment in the software package, called koopmans, are described in a new and comprehensive article by MARVEL researchers at EPFL and PSI [4]. We have extended the range of applicability of the approach by developing a non-collinear formulation of the Koopmans spectral functional based on Wannier functions and density-functional perturbation. This allows calculating accurate band structures in the presence of SOC and possibly non-collinear magnetism. This advance has been implemented in the KCW package of QE and it is currently under extensive testing. In Fig. 2, we report a validation of the theory and implementation for the band structure of $CsPbBr_3$ (one member of the family of halide perovskites, excellent candidates for optoelectronic applications) with and without SOC. The predicted band gap with SOC is of 1.81 eV and compares very well with the experimental gap of 1.85 eV and state-of-the-art many-body perturbation theory results [5].

1.2 AiiDAlab

The nanotech@surfaces laboratory at Empa collaborates with experimental partners to address scientific inquiries focused on two key areas: investigating point defects in 2D transition metal dichalcogenides and characterizing the magnetic properties of graphene-based low dimensional nanomaterials, including those with transition metal elements. Key point in this research field are our efforts in enhancing the AiiDAlab QEapp[1] with new features. Notably, we have enabled the QEapp with the possibility to treat 1D and 2D materials. In addition, charged systems can be now treated, spin-orbit coupling effects can be included as well as Hubbard corrections. The progress in the QEapp has significantly contributed to ongoing research at Empa. Our modified

[1] https://github.com/aiidalab/aiidalab-qe/tree/empa_qeapp



	Method	Gap (eV)
noSOC	G_0W_0	2.56
	KI@LDA	3.28
	qsGW	3.15
SOC	G_0W_0	1.31
	KI@LDA	**1.81**
	qsGW$^{(+)}$	2.03
	Exp$^{(*)}$	**1.85**

Figure 2: *Band structure of $CsPbBr_3$ in its high-temperature cubic phase obtained with the non-collinear KCW code as a one-shot correction on top of LDA. Bands are calculate both with and without the inclusion of SOC. $(^*)$ The experimental value is corrected to remove finite temperature effect (not included in the theory). $(^+)$ SOC effects for the quasi-particle self-consistent GW (qsGW) results are computed at G_0W_0 level.*

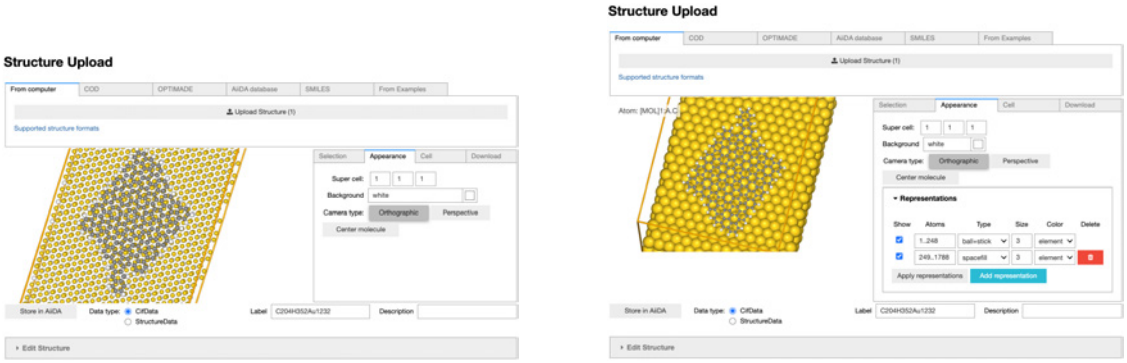


Figure 3: *AiiDAlab structure viewer. Left: The old version; it was inconvenient to use for large structures as it did not allow to specify different representations. Right: The new version with representation feature. The users can select a sub-part of a system and configure its view.*

QEapp has been instrumental in investigating the electronic and magnetic properties of laterally porphyrin-fused zigzag nanoribbons, with a forthcoming publication. Simultaneously, we are exploring the electronic properties of a Re dopant and a Sulfur vacancy in MoS_2. The latest release of the QEapp integrates some of these features, such as periodicity and charge, with an ongoing commitment to introducing new functionalities. The plugin implementation of the QEapp streamlines the integration of features, exemplified by the collaboration between PSI and Empa. This collaboration focuses on integrating `aiida-vibroscopy`[2] workflows into the QEapp, enhancing its capabilities further.

a) *Structure viewer* The default viewer had limitations in representing structures with flexibility, as illustrated in Fig. 3 (left). In response to user feedback requesting custom representations, a significant focus over the past year has been to address this need by introducing the concept of representations to the viewer. This enhancement allows users to break down a structure into multiple substructures and display them in distinct ways, as depicted in Fig. 3 (right). This feature proves especially useful when dealing with large structures such as organic molecules adsorbed on a substrate.

b) *FLEXPART-COSMO* We are actively assisting various groups at Empa in adopting AiiDA/AiiDAlab, and one notable project involves collaboration with Stephan Henne from the Laboratory for Air Pollution/Environmental Technology. Since August 2023, Lucas Fernandes Vilanova has joined the project to carry on the implementation of the FLEXPART-COSMO workflow, which aims to automate daily simulation runs in the laboratory.

c) *CSCS-MFA app* As the threat of unauthorized access to supercomputer centers grows, there has been a concerted effort to enhance security measures. These measures pose chal-

[2] https://github.com/mikibonacci/aiidalab-qe-vibroscopy

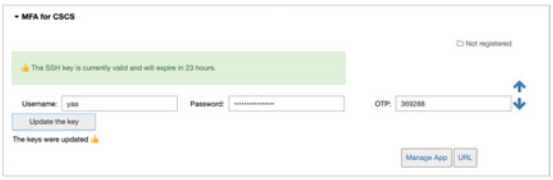


Figure 4: *MFA CSCS app allows for a quick and easy key update using multi-factor authentication.*

lenges for workflow managers like AiiDA that rely on seamless, user-free access to supercomputer centers. To address these challenges, we have developed a user-friendly AiiDAlab application (Fig. 4) aimed at simplifying the setup of SSH connections for AiiDAlab users. Essentially, users only need to input their username, password, and a 6-digit number obtained from an authentication app (like Google Authenticator) to grant access to the supercomputing infrastructures for up to 7 days. After that period the user has to provide a new authentication code.

d) *Surfaces app: new features* We have implemented significant updates to the AiiDAlab Surfaces app[3]. Notably, we merged the scanning probe microscopy (SPM) app into the Surfaces app, streamlining and enhancing its functionality. The interface for various types of SPM simulations has been unified to provide a more seamless user experience. Additionally, a new feature has been introduced, enabling users to compute the adsorption energy of molecules on surfaces.
Furthermore, we have made improvements to the resource handling model. In previous versions, workflows would automatically select the appropriate resources, which proved problematic as it was highly specific to a machine and often resulted in unexpected behavior. To address this, we have adopted a suggestion model. Under this approach, the automated tool suggests the required amount of resources, giving users the flexibility to override these values before submission.

e) *Documentation* Effective documentation plays a crucial role in fostering community growth. In the context of AiiDAlab, we maintain two types of documentation: (i) a comprehensive guide[4] covering the needs for general users, deployment guidelines, and app development, and (ii) a documentation specific to the base widgets[5], which is tailored for app developers. To ensure the consistent expansion and quality of our documentation, we have implemented monthly AiiDAlab documentation days.

f) *Publications* In 2023 AiiDAlab tools at Empa were employed mainly for the characterization of the electronic and magnetic properties of carbon based nanomaterials [6, 7, 8, 9][13].

2 Contribution to overall goals and initial proposal

The establishment of the Laboratory for Materials Simulations at PSI, accompanied by the recruitment of two group leaders (Giovanni Pizzi and Michael Schüler) and two tenure-track scientists (Nicola Colonna and Iurii Timrov), and several PhD students and postdocs at PSI and Empa, strategically aligns with the objectives of phase III for Pillar 4. The computational tools and advances described in this report, their implementation in widely-used open-source codes, and their deployment as turnkey solutions through automated and robust AiiDA workflows and AiiDAlab apps represent a step further toward a computational infrastructure for reliable spectroscopy simulations in core areas of interests for PSI and Empa. This together with the strengthened and efficient collaboration with experimental groups at both institutions (see section below) is fully in line with the final goal of permanently integrating MARVEL into the Swiss scientific landscape, and contribute to fortifying materials science in Switzerland and globally.

3 Collaborative and interdisciplinary components

A new scientific collaboration between the Spectroscopy of Quantum Materials group (in particular with Vladimir Strokov and collaborators) and the Laboratory of Materials Simulations has been recently established to complement ARPES measurements of the band structure of strained Germanium quantum dots with *ab initio* simulations. The efforts on the non-collinear extension of Koopmans functional is taking place in close collaboration with Antimo Marrazzo from the University of Trieste.
A collaborative working group has been established between the Neutron and Muon division of PSI and the Laboratory of Materials Simulations, focusing on cooperative efforts in modeling magnons through model Hamiltonians and investigating muon rest sites in

[3] https://github.com/nanotech-empa/aiidalab-empa-surfaces
[4] https://aiidalab.readthedocs.io
[5] https://aiidalab-widgets-base.readthedocs.io

selected materials. Concurrently, vibrational spectroscopy initiatives encompass a partnership with the University of Bremen [10]. In addition, collaborative efforts in XPS and XAS are underway, closely intertwined with the H2020 project BIG-MAP (a constituent of Battery 2030+), and Deborah Prezzi's team at the University of Modena.

In addition to the collaboration with Empa experimentalists active in the characterization of 0D, 1D, and 2D materials, we started a collaboration with the Univeristy of Rome (Marco Di Giovannantonio) to enable the use of AiiDAlab apps for the supercomputer hosted at CINECA. Collaboration with IBM in Zurich (Leonard Lieske) is also centered on offering access to AiiDAlab for experimentalists interested in performing simulations in parallel to experiments. Collaboration with Jan Wilhelm (Regensburg) is aimed to design AiiDAlab applications leveraging upcoming GW capabilities of the CP2K code for 2D materials.

At present, AiiDAlab instruments target experimentalists with experience in collaborating with theoreticians. For persons interested in testing the platform, we typically ask to describe the type of calculations they would like to perform and for which class of systems. If the available AiiDAlab tools cover the cases specified, we organize a three to four days tutorial with examples. After this, we provide assistance to submit production simulations till the researchers are confident enough with the procedures. The feedback obtained during the collaboration is precious input to improve/complement the AiiDAlab tools. In case the simulations foreseen by the experimentalists require the creation of new AiiDAlab tools (as in the case of defects in 2D materials) a collaboration could start with the aim to create them with direct inputs from the experimentalists for a better design.

MARVEL publications

List of publications either resulting directly from the NCCR (marked with a red hexagon) or with minor contributions from the NCCR.

- [1] M. dos Santos Dias, N. Biniskos, F. J. dos Santos, K. Schmalzl, J. Persson, F. Bourdarot, N. Marzari, S. Blügel, T. Brückel, and S. Lounis, *Topological magnons driven by the Dzyaloshinskii-Moriya interaction in the centrosymmetric ferromagnet Mn_5Ge_3*, Nature Communications **14**, 7321 (2023).
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- [4] E. Linscott, N. Colonna, R. De Gennaro, N. L. Nguyen, G. Borghi, A. Ferretti, I. Dabo, and N. Marzari, *koopmans: An Open-Source Package for Accurately and Efficiently Predicting Spectral Properties with Koopmans Functionals*, Journal of Chemical Theory and Computation **19**, 7097 (2023).
- [5] J. Wiktor, U. Röthlisberger, and A. Pasquarello, *Predictive determination of band gaps of inorganic halide perovskites*, The Journal of Physical Chemistry Letters **8**, 5507 (2017).
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List of year 10 publications related to Pillar 4

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Magnetostriction-Driven Muon Localization in an Antiferromagnetic Oxide
Physical Review Letters **132**, 046701 (2024).
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:8s-qh

○ M. Bommert, B. Schuler, C. A. Pignedoli, R. Widmer, and O. Gröning
Ambipolar charge transfer of larger fullerenes enabled by the modulated surface potential of h-BN/Rh(111)
Carbon **216**, 118592 (2024).
Group(s): Pignedoli / Project(s): P4
Links to article: Journal / Open access
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How to verify the precision of density-functional-theory implementations via reproducible and universal workflows
Nature Reviews Physics **6**, 45 (2024).
Group(s): Marzari, Pizzi / Project(s): P3, P4
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⬢○ G. Gebreyesus, L. Bastonero, M. Kotiuga, N. Marzari, and I. Timrov
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Physical Review B **108**, 235171 (2023).
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⬢○ E. Linscott, N. Colonna, R. De Gennaro, N. L. Nguyen, G. Borghi, A. Ferretti, I. Dabo, and N. Marzari
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Advanced Simulation Methods

From Materials to Devices

Project leaders: Philipp Werner (UniFR), **Mathieu Luisier** (ETH Zurich), **Daniele Passerone** (Empa)

Partner: Michael Schüler (PSI and UniFR)

1 Progress of the different efforts

1.1 *Ab initio* multi-tier GW+DMFT

Ruslan Mushkaev, the MARVEL funded PhD student in the Werner group at UniFR has familiarized himself with the *ab initio* multi-tier GW+DMFT framework [2] in a project focused on the perovskite compounds $SrVO_3$, $SrCrO_3$ and $SrMnO_3$. The goal of this project was to test the robustness and predictive power of the multi-tier approach, which treats the high, intermediate and low-energy subspaces at the G_0W_0, self-consistent GW, and extended DMFT (EDMFT) level, respectively, by comparing the results for different intermediate and low-energy subspaces. Specifically, the following three combinations for the (intermediate, low-energy) spaces have been considered: (i) (t_{2g}, t_{2g}), (ii) ($t_{2g} + e_g$, $t_{2g} + e_g$), and (iii) (t_{2g}+(oxygen)p, t_{2g}) orbitals. More or less consistent results were obtained for the mass enhancements and spectral functions, which shows that the multi-tier GW+DMFT framework is internally consistent. Ruslan Mushkaev also studied the spin-excitation spectra and electron energy loss spectra (EELS) using a postprocessing approach based on the random phase approximation.

In separate work by PhD student Viktor Christiansson, the GW, DMFT, EDMFT and GW+EDMFT frameworks were used to investigate the electronic structure of the recently discovered bi-layer nickelate superconductor $La_3Ni_2O_7$ [11]. Also here, the charge susceptibility was computed and it was found that the system is close to an instability towards the formation of incommensurate stripe order, Fig. 1 [1].

We also performed an *ab initio* study of the purported room-temperature superconductor LK-99 [12], which created a remarkable, but short-lived hype in the condensed matter community and beyond. Our analysis suggested that this system is too strongly correlated to be a high-temperature superconductor [13].

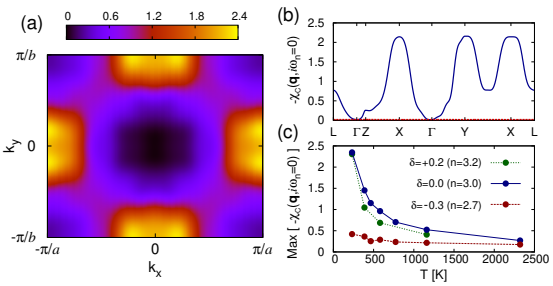

Figure 1: *Charge susceptibility $-\chi_c(\mathbf{q}, i\omega_n = 0)$ of $La_3Ni_2O_7$ at $\beta = 50\ eV^{-1}$ from GW+DMFT (a) in the $\mathbf{k}_z = 0$ plane for $d_{x^2-y^2}$ and (b) along the indicated high-symmetry path. (c) Temperature and doping dependence of the maximum of $-\chi_c(\mathbf{q}, i\omega_n = 0)$ (from [1]).*

1.2 Electrical, thermal, and optical transport in 2D materials

Two members of the ETH Zurich team of Mathieu Luisier left MARVEL after either finishing their PhD (Guido Gandus) or completing their postdoc (Youseung Lee). They both joined semiconductor companies where they remain active in the field of nano-device modeling.

In terms of research, progress has been made on several fronts involving the OMEN code, a quantum transport solver relying on the non-equilibrium Green's function (NEGF) formalism. First, the electron-phonon interaction model of OMEN has been improved to account for the non-diagonal entries of the scattering self-energies. Typically, these entries are neglected, which can lead to an underestimation of the influence of phonons on the electron population. Including these elements up to a predefined cut-off radius required to modify the way the scattering self-energies are computed. Since the latter operation is time consuming, it was ported to GPUs. This upgrade has been used to calculate the mobility of monolayer MoS_2 and to compare it with results obtained with the linearized Boltzmann transport equation (LBTE) where no cut-off radius is applied to the electron-phonon interactions. Excellent agreement between both methods was obtained (Fig. 2a). This sanity check validates the implemented approach. The NEGF solver can go beyond mobility calculations and shed light on the behavior of de-

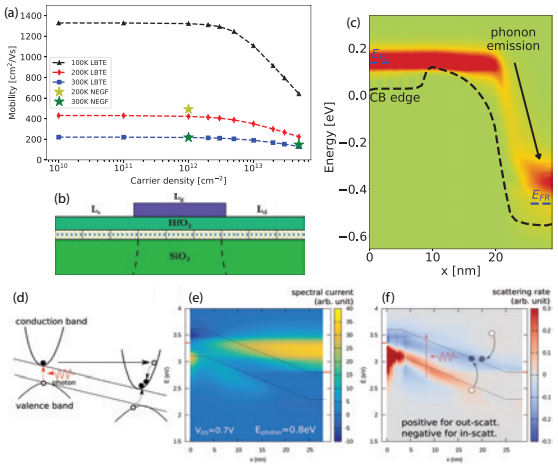

Figure 2: *(a) Monolayer MoS_2 mobility as a function of the electron density and temperature as calculated with LBTE (lines with symbols) and with NEGF (stars). (b) Schematic view of a single-gate MoS_2 field-effect transistor (FET) deposited on a SiO_2 substrate and using a HfO_2 dielectric. (c) Spectral current distribution in the ON-state of the FET in (b). Red indicates high current concentrations, green no current. The dashed line represents the conduction band edge. (d) Schematic illustration of the photon-induced avalanche multiplication process encountered in avalanche photo-diode. (e) Spectral current and (f) local in-/out-scattering rates in a bulk InAs structure under a single photon energy illumination ($\hbar\omega = 0.8$ eV).*

vices, e.g., MoS_2 single-gate field-effect transistors (Fig. 2b). Such simulations do not only return the "current vs voltage" characteristics of transistors, but also the distribution of the current along their channel as a function of the electron energy (Fig. 2c). Obviously, significant energy losses occur close to the drain side, where the electric field is the highest.
Work has also been undertaken at ETH Zurich to enable the modeling of nano-devices in the presence of electron-electron interactions within the GW approximation [3, 4], thus establishing a link with UniFR. This level of complexity is needed, for example, to capture avalanche multiplication processes, which can be triggered by the absorption of a photon that generates an electron-hole pair (Fig. 2d). The application of an external bias then accelerates both particles which, through impact ionization, create additional carriers. By combining electron-electron and electron-photon interactions through dedicated scattering self-energies, photon-induced avalanche processes could be simulated within a bulk InAs structure. The resulting spectral distribution of the electron and hole currents as well as the in- and out-scattering rates are presented in Figs. 2e and 2f, respectively. They clearly indicate that the photon-generated carriers get multiplied once they are accelerated by the underlying electric field.
Finally, the ETH Zurich team published an invited paper [5] and book chapter [6] that discuss the state-of-the-art in *ab initio* device simulation based on NEGF.

1.3 *Ab initio* Wannier-function approach to excitons

In the Schüler group, the MARVEL-funded PhD student Gian Parusa started at the beginning of the year and familiarized< himself with first-principle approaches to angle-resolved photoemission spectroscopy (ARPES). He has already obtained optimized pseudopotentials to accurately describe photoelectron states — an essential step toward implementing efficient and accurate ARPES calculations. These activities tie directly into MARVEL Pillar 4 (Long-term Integration in the Swiss Scientific Landscape), as we are preparing collaborations with experimentalists at PSI. We also connect to MARVEL Pillar 3 (Digital Infrastructure of Open Simulations and Data) in our efforts to automatize the construction of these pseudopotentials in collaboration with Giovanni Pizzi.
In collaboration with Philipp Werner and his PhD student Viktor Christiansson, we have further developed an *ab initio* method to describe excitons out of equilibrium. With the first-principle Coulomb interactions provided by Viktor Christiansson we have performed G_0W_0 calculations and solved the Bethe-Salpeter equation (BSE) for the excitons directly in the Wannier basis with unprecedented speed. Based on this method and in close collaboration with leading experimentalists, we have revealed how the Berry curvature of 2D materials can be extracted from the exciton signal in time-resolved ARPES [7] (Fig. 3).
The second PhD student Juan Felipe Pulgarin is continuing this line of research with systematic benchmarks. We expect that the efficiency of the Wannier-GW method can be combined with non-equilibrium simulations of materials and facilitate the scaling up to devices, which is a synergy with the efforts at ETH Zurich.

1.4 Beyond-DFT modeling of electronic properties and transport in realistic systems

At Empa, in the Passerone group, the MARVEL-funded postdoc Anooja Jayaraj has started at the beginning of the year and got acquainted with the massive palette of methods left by Guido Gandus, i.e., a fully acces-

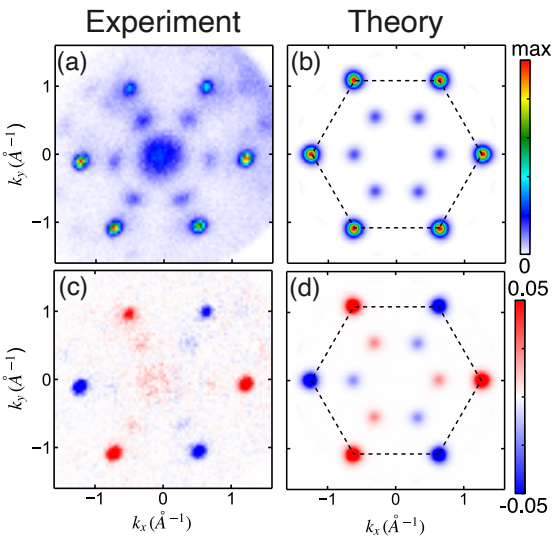

Figure 3: *Wannier-BSE vs experiments. (a) and (b) Polarization-averaged time-resolved ARPES signature of excitons in monolayer WSe_2, comparing experiment (a) and theory (b). (c) and (d) Circular dichroism with respect to the pump pulse polarization from experiments (c) and our calculation (d). The positive-negative pattern of the dichroism in (c) and (d) directly reflects the Berry curvature in each valley.*

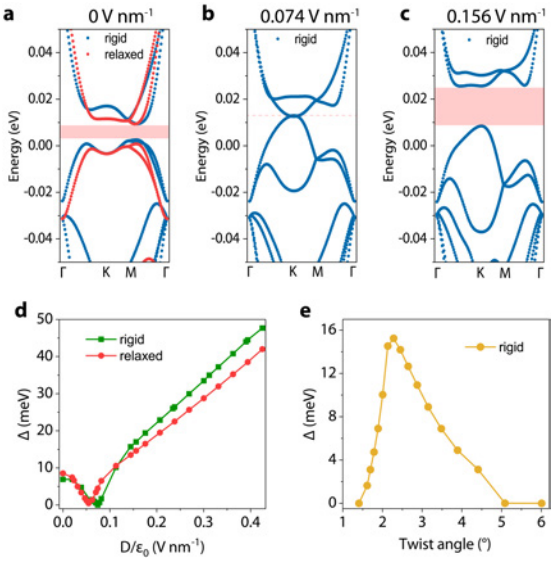

Figure 4: *(a) Band structure of TDTLG with θ = 1.8 degrees in the absence of an external electric field. The blue (orange) lines denote the bands of unrelaxed (relaxed) TDTLG. (b, c) Calculated band structure in the presence of an external field. The displacement field D has been calculated using the dielectric constant of h-BN and screening effects have been ignored. (d) Band gap as a function of D for both the relaxed (orange curve) and unrelaxed (green curve) structure of TDTLG. (e) Band gap as a function of twist angle for unrelaxed TDTLG in the absence of an external displacement field.*

sible, open source and versatile suite of programs for quantum transport (qtpyt) and correlated systems based on exact diagonalization and DMFT (edpyt). She is now applying the DMFT+NEGF approach to the simulation of Coulomb blockade effects in quantum-dot transport regime observed experimentally in the Empa laboratories nanotech@surfaces and Transport at Nanoscale Interfaces. The approach originally developed by Guido Gandus, where the "active correlated" region is modeled via a system of multiple impurity Anderson models, also requires a parallelization effort in the original edpyt code to afford the modeling of realistic quantum systems.

Anooja Jayaraj together with the experimental group led by Mickael Perrin at Empa could already complete the first publication which is presently under review. The topic is twisted trilayer graphenes. Twisted van der Waals heterostructures have emerged as a versatile, tunable platform for the exploration of magnetotransport and optoelectronic properties. This work considers the theoretical counterpart to the experimental realization of the scarcely explored twisted double trilayer graphene (TDTLG) devices. Due to unit cell sizes with ∼13'000 atoms, tight-binding calculations were used to calculate the band structure and rationalize the experimentally observed charge-transport behavior. The Hamiltonian was built using orbital distance-dependent Slater-Koster parameters as implemented in WannierTools. This work also explores the configuration space of the stacking order in TDTLG in order to verify the stacking order of the fabricated device. Lattice relaxation is found to have a negligible effect on the band structure of TDTLG at the fabricated twist angle of θ = 1.8 degrees. Band structure calculations show the range of twist angles for which TDTLG is predicted to be intrinsically insulating. The effect of an externally applied electric field on the band-gap of ABC–ABC stacked trilayer graphene demonstrates the semi-metal-instulator-semi-metal transition that is observed experimentally using resistivity measurements (Fig. 4). The band structure in the presence of the external field is used to explain the semi-metal-insulator-semi-metal transition. It is further used to eliminate other stacking possibilities such as ABA–ABC and ABA–ABA and narrow the stacking configuration to ABC–ABC or CAB–ABC, since an experimental characterization of the stacking order within a fabricated device is difficult.

Four important papers in collaboration with

experimental groups on the cotunneling simulation of molecules on surfaces [8] as well as the simulation of electronic transport in nanoribbon-based devices [9, 10], together with another paper about the GW approach developed by Guido Gandus during his thesis [3], have been published in 2023.

2 Contribution to overall goals and initial proposal

The work at ETH Zurich continues to progress according to the proposal for MARVEL's phase III. The focus is set on the development of advanced, *ab initio* models to simulate electrical, optical, and thermal effects in nanoscale devices. During year 10, a new feature was added, photon-induced avalanche processes. Furthermore, the electron-phonon scattering model of OMEN was improved.
The goal of the MARVEL phase III effort in UniFR is to develop a user-friendly GW+EDMFT simulation framework for correlated materials. In year 10, we have systematically tested this method on a range of compounds with perovskite structure. Work to connect the simulation framework to the QUANTUM ESPRESSO *ab initio* code is under way.

3 Collaborative and interdisciplinary components

The ETH Zurich and Empa groups actively collaborate on the simulation of 2D materials and on the inclusion of correlation effects in these investigations. Both teams work with scientists from Pillar 3 to automatize their calculations with AiiDA and define appropriate simulation workflows. The PSI and UniFR groups collaborate with experimentalists at PSI on ARPES and resonant inelastic X-ray scattering (RIXS), and they were both involved in a project related to excitons. The ETH Zurich, Empa, PSI and UniFR groups will intensify their collaboration from year 10 onward to extend the modeling of correlation effects from the materials to the device level, and from equilibrium to non-equilibrium conditions.

MARVEL publications

List of publications either resulting directly from the NCCR (marked with a red hexagon) or with minor contributions from the NCCR.

[1] V. Christiansson, F. Petocchi, and P. Werner, *Correlated electronic structure of $La_3Ni_2O_7$ under pressure*, Physical Review Letters **131**, 206501 (2023).

[2] F. Nilsson, L. Boehnke, P. Werner, and F. Aryasetiawan, *Multitier self-consistent GW + EDMFT*, Physical Review Materials **1**, 043803 (2017).

[3] G. Gandus, Y. Lee, L. Deuschle, D. Passerone, and M. Luisier, *Efficient and accurate defect level modeling in monolayer MoS_2 via GW+DFT with open boundary conditions*, Solid-State Electronics **199**, 108499 (2023).

[4] G. Gandus, J. Cao, T. Agarwal, M. Luisier, and Y. Lee, *Ab initio quantum transport simulations of defective devices based on 2-D materials via a projected-GW approach*, in *2022 International Electron Devices Meeting (IEDM)* (IEEE, Piscataway, NJ, USA, 2022), pp. 28.3.1–28.3.4.

[5] Y. Lee, J. Cao, and M. Luisier, *Atomistic Simulation of Nanoscale Devices*, IEEE Nanotechnology Magazine **17**, 4 (2023).

[6] M. Luisier, C. Klinkert, S. Fiore, J. Backman, Y. Lee, C. Stieger, and S. Àron, *Field-Effect Transistors Based on 2D Materials: A Modeling Perspective*, in *Beyond-CMOS: State of the Art and Trends*, A. Cresti, ed. (Wiley-ISTE, 2023), pp. 33–78.

[7] 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*, arXiv:2308.09634 (2023).

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

[9] W. Huang, O. Braun, D. I. Indolese, G. Borin Barin, G. Gandus, M. Stiefel, A. Olziersky, K. Müllen, M. Luisier, D. Passerone, P. Ruffieux, C. Schönenberger, K. Watanabe, T. Taniguchi, R. Fasel, J. Zhang, M. Calame, and M. L. Perrin, *Edge Contacts to Atomically Precise Graphene Nanoribbons*, ACS Nano **17**, 18706 (2023).

[10] C. Hsu, M. Rohde, G. Borin Barin, G. Gandus, D. Passerone, M. Luisier, P. Ruffieux, R. Fasel, H. S. J. van der Zant, and M. El Abbassi, *Platinum contacts for 9-atom-wide armchair graphene nanoribbons*, Applied Physics Letters **122**, 173104 (2023).

Other references

[11] H. Sun, M. Huo, X. Hu, J. Li, Y. Han, L. Tang, Z. Mao, P. Yang, B. Wang, J. Cheng, D.-X. Yao, G.-M. Zhang, and M. Wang, *Signatures of superconductivity near 80 K in a nickelate under high pressure*, Nature **621**, 493 (2023).

[12] S. Lee, J. Kim, H.-T. Kim, S. Im, S.-M. An, and K. H. Auh, *Superconductor $Pb_{10-x}Cu_x(PO_4)_6O$ showing levitation at room temperature and atmospheric pressure and mechanism*, arXiv:2307.12037 (2023).

[13] C. Yue, V. Christiansson, and P. Werner, *Correlated electronic structure of $Pb_{10-x}Cu_x(PO_4)_6O$*, arXiv:2308.04976 (2023).

List of year 10 publications related to Advanced Simulation Methods

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).

○ C.-Y. Cheon, Z. Sun, J. Cao, J. F. G. Marin, M. Tripathi, K. Watanabe, T. Taniguchi, M. Luisier, and A. Kis
Disorder-induced bulk photovoltaic effect in a centrosymmetric van der Waals material
npj 2D Materials and Applications **7**, 74 (2023).
Group(s): Luisier / Project(s): ASM
Links to article: Journal / Open access
Related datasets: not applicable

⬢○ N. Krane, E. Turco, A. Bernhardt, D. Jacob, G. Gandus, D. Passerone, M. Luisier, M. Juríček, R. Fasel, J. Fernández-Rossier, and P. Ruffieux
Exchange Interactions and Intermolecular Hybridization in a Spin-1/2 Nanographene Dimer
Nano Letters **23**, 9353 (2023).
Group(s): Luisier, Passerone / Project(s): ASM
Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.8128962

⬢○ W. Huang, O. Braun, D. I. Indolese, G. Borin Barin, G. Gandus, M. Stiefel, A. Olziersky, K. Müllen, M. Luisier, D. Passerone, P. Ruffieux, C. Schönenberger, K. Watanabe, T. Taniguchi, R. Fasel, J. Zhang, M. Calame, and M. L. Perrin
Edge Contacts to Atomically Precise Graphene Nanoribbons
ACS Nano **17**, 18706 (2023).
Group(s): Luisier, Passerone / Project(s): ASM
Links to article: Journal / Open access
Related datasets: not applicable

Z. Cheng, J. Backman, H. Zhang, H. Abuzaid, G. Li, Y. Yu, L. Cao, A. V. Davydov, M. Luisier, C. A. Richter, and A. D. Franklin
Distinct Contact Scaling Effects in MoS_2 Transistors Revealed with Asymmetrical Contact Measurements
Advanced Materials **35**, 202210916 (2023).
Group(s): Luisier / Project(s): ASM
Links to article: Journal / Open access (embargo 27.02.2024)
Related datasets: not applicable

⬢○ C. Hsu, M. Rohde, G. Borin Barin, G. Gandus, D. Passerone, M. Luisier, P. Ruffieux, R. Fasel, H. S. J. van der Zant, and M. El Abbassi
Platinum contacts for 9-atom-wide armchair graphene nanoribbons
Applied Physics Letters **122**, 173104 (2023).
Group(s): Luisier, Passerone / Project(s): ASM
Links to article: Journal / Open access
Related datasets: not applicable

⬢○ Y. Lee, J. Cao, and M. Luisier
Atomistic Simulation of Nanoscale Devices
IEEE Nanotechnology Magazine **17**, 4 (2023).
Group(s): Luisier / Project(s): ASM
Links to article: Journal / Open access
Related datasets: not applicable (review article)

○ V. Christiansson, F. Petocchi, and P. Werner
Correlated electronic structure of $La_3Ni_2O_7$ under pressure
Physical Review Letters **131**, 206501 (2023).
Group(s): Werner / Project(s): ASM
Links to article: Journal / Open access
Related datasets: not applicable

○ F. Petocchi, J. Chen, J. Li, M. Eckstein, and P. Werner
Photoinduced charge dynamics in $1T-TaS_2$
Physical Review B **107**, 165102 (2023).
Group(s): Werner / Project(s): ASM
Links to article: Journal / Open access
Related datasets: not applicable

M. Luisier, C. Klinkert, S. Fiore, J. Backman, Y. Lee, C. Stieger, and S. Àron
Field-Effect Transistors Based on 2D Materials: A Modeling Perspective
in *Beyond-CMOS: State of the Art and Trends*, A. Cresti, ed. (Wiley-ISTE, 2023), pp. 33–78.
Group(s): Luisier / Project(s): ASM
Links to article: Book / Open access (submitted version)
Related datasets: not applicable (review article)

⬢○ 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
arXiv:2308.09634 (2023).
Group(s): Schüler, Werner / Project(s): ASM
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:zq-tj

- J. Chen, F. Petocchi, V. Christiansson, and P. Werner
  Nature of the photo-induced metallic state in monoclinic VO_2
  arXiv:2310.18195 (2023).
  Group(s): Werner / Project(s): ASM

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

- V. Christiansson and P. Werner
  Quaternary borocarbides: a testbed for DFT for superconductors
  arXiv:2310.03723 (2023).
  Group(s): Werner / Project(s): ASM

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

Quantum Simulations

Leveraging Quantum Computers and Algorithms for Materials Discovery

Project leader: Giuseppe Carleo (EPFL)

Partners: Jürg Hutter (UZH), **Ivano Tavernelli** (IBM), **Zoë Holmes** (EPFL)

1 Progress of the different efforts

The goal of the Quantum Simulations project is to close the gap between classical and quantum computing in order to enable more accurate electronic structure calculations that are currently unattainable with classical computing alone. To achieve this, the project aims to develop new hybrid quantum algorithms that combine the strengths of both classical and quantum computing, as well as algorithmic tools that interface with classical electronic structure tools. In addition, the project aims to research and develop a quantum machine learning pipeline that uses wavefunctions to classify materials and their properties.
The following are the three interconnected goals of the project.

- Develop new hybrid quantum algorithms that leverage advanced machine learning and optimization techniques in order to overcome the limitations of current quantum hardware.
- Research and develop algorithmic tools that interface with state-of-the-art classical electronic structure tools in order to design suitable problems for quantum hardware.
- Develop a quantum machine learning pipeline that uses wavefunctions for material classification and property prediction.

1.1 Description of the project progress

In year 10 we developed the core methods initially conceptualized in year 9 after a thorough evaluation of quantum resources. This progress involved the refinement of various techniques, including but not limited to, the integration of machine learning, circuit cutting methodologies, and adaptive circuits. These endeavors were undertaken to extend the capabilities of near-term hardware. In addition, we have coordinated a large community effort to analyze existing variational methods, both classical and quantum, to come to a consensus on a metric for accuracy (Fig. 1) [1].

a) *Hybrid quantum-classical variational ansatz* Last year we reported the introduction of a completely variational ansatz combining a neural network and a parameterized quantum circuit in order to determine the ground state of quantum systems. The performances of this new method were initially assessed on spin systems. During this year, we first extended the combined method to other classical variational ansatzes, such as mean field and Jastrow. Then, we focused on the study of molecular systems, in particular configurations in which the static correlation effects are enhanced by the stretching of interatomic bonds. We recently reported the results of our experiments in a preprint [2]. Stefano Barison, PhD student in the Carleo group, is working on this project.

b) *Hybrid quantum-classical periodic embedding* The interface between the classical electronic structure code CP2K and IBM's Qiskit Nature library[1] is finished and officially released in both software. There are now three ways in which data can be exchanged between them: formatted files on disk, binary files on disk, and via UNIX/INET sockets. We have implemented a classical-quantum embedding approach that was used in a previous study [6], and extended it to support periodic boundary conditions, thereby enabling the simulation of localized defects in materials and providing access to the properties of both ground and excited electronic states. The implementation has been extensively tested on small molecular systems at different correlation regimes. Currently, simulations of optically addressable defects in monolayer hexagonal boron nitride (V_B^- defect in h-BN) and bulk magnesium oxide (F-center in MgO) are underway. Stefano Battaglia, postdoc in the Hutter group, and Max Rossmannek, PhD student in the Tavernelli group, are working on this project.

c) *Real-time dynamics of quantum systems with circuit knitting* Simulating the dynamics of large quantum systems is a formidable yet vital pursuit for obtaining a deeper understand-

[1] https://github.com/qiskit-community/qiskit-nature/tree/stable/0.5

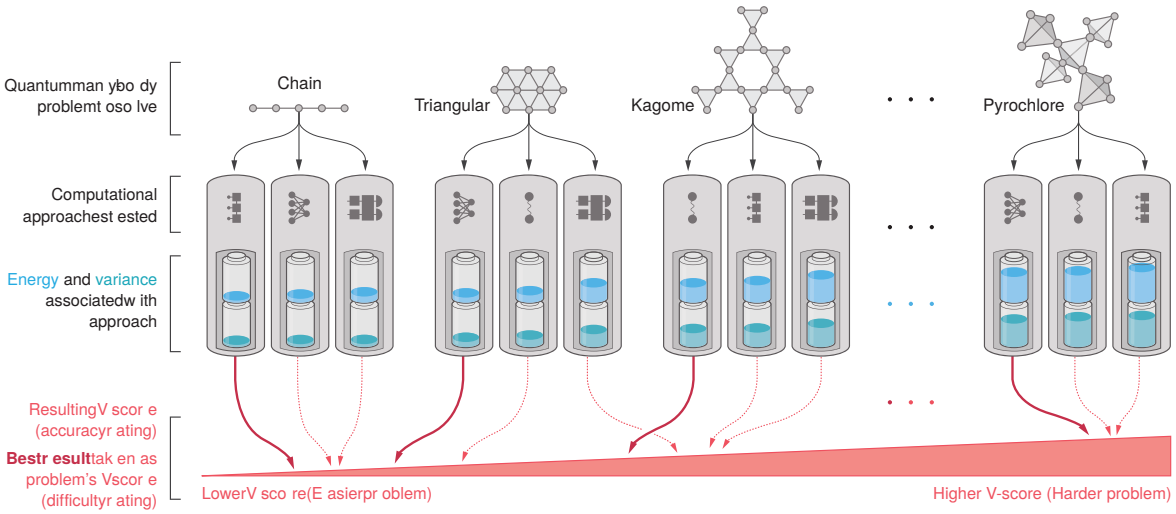

Figure 1: *The study performed in [1] provides a comprehensive collection of computational outcomes for quantum many-body ground-state problems. For each Hamiltonian in the dataset, the mean energy and its variance are computed utilizing various variational techniques, including physically motivated ansatzes, neural networks, tensor networks, and parameterized quantum circuits. The energy and the variance are integrated into the V-score, a metric of variational accuracy. A low V-score indicates high accuracy. The V-score is then employed to prioritize the Hamiltonians in terms of simulation precision, identifying which quantum many-body models are challenging to simulate using present techniques.*

ing of quantum mechanical phenomena.While quantum computers hold great promise for speeding up such simulations, their practical application remains hindered by limited scale and pervasive noise. In our recent preprint [3], we propose an approach that addresses these challenges by employing circuit knitting [7, 8, 9] to partition a large quantum system into smaller subsystems that can each be simulated on a separate device. The evolution of the system is governed by the projected variational quantum dynamics (PVQD) algorithm [10], supplemented with constraints on the parameters of the variational quantum circuit, ensuring that the sampling overhead imposed by the circuit knitting scheme remains controllable. We test our method on quantum spin systems with multiple weakly entangled blocks each consisting of strongly correlated spins, where we are able to accurately simulate the dynamics while keeping the sampling overhead manageable. Further, we show that the same method can be used to reduce the circuit depth by cutting long-ranged gates. This research has been performed by Gian Gentinetta and Friederike Metz in the group of Giuseppe Carleo and will be presented in a talk at the quantum techniques for machine learning (QTML) conference in November 2023 at CERN.

d) *Real-time dynamics of quantum systems with adaptive methods* While circuit knitting techniques address the spatial-like limitations of current hardware, qubit decoherence times and operation infidelities require us to optimize also the circuit depth. For this reason we introduced an adaptive scheme for the PVQD algorithm [10]. Instead of fixing a variational quantum circuit at the beginning of the simulation, we define a pool of gates, depending on the Hamiltonian governing the physical system. When the optimization of the variational parameters fails to converge below the infidelity threshold, we choose a new gate from the pool to grow the circuit. This is accomplished by looking for the gate that maximizes infidelity decrement, as proposed for ground-state search in [11], and can be performed in parallel on multiple quantum processors. We tested the method on driven spin chains and fermionic lattice systems. Recently, we reported the results in a preprint [4]. Stefano Barison worked on this project together with David Linteau, a Master's student in the Carleo group.

e) *Continuous-Space Quantum Simulation* Most quantum many-body systems including those of electronic structure and materials are natively described in first quantization. However, simulating continuous-space systems on quantum computers is challenging as the systems have to be discretized and mapped onto qubits while respecting the underlying exchange statistics. The discretization usually amounts to either discretizing space itself or choosing a suitable finite basis set which

introduces errors and scales poorly with the number of particles. In this work, we propose an alternative approach of harnessing quantum resources within variational Monte Carlo simulations for continuous-space problems which does not require any form of discretization. To that end, the wavefunction ansatz is partly represented by a parameterized quantum circuit and optimized similarly to the neural quantum states framework [12]. We have applied our hybrid quantum-classical algorithm to the paradigmatic 1D quantum rotor model [13] and showed how the accuracy of the ground-state energy can be controlled by the circuit depth. The results were compared to typical classical ansatzes such as Jastrow wavefunctions and MPS calculations on a discretized approximation of the model. In terms of the latter, we have demonstrated a reduction in the number of qubits when simulating the system using our continuous-space formalism. We are currently working on extending the framework to fermionic systems. Friederike Metz is working on this project.

f) *Quantum machine learning from quantum data for material characterization* Recently, there has been a growing interest in the intersection of quantum computing and artificial intelligence, leading to the emergence of quantum convolutional neural networks (QCNNs) [14] [5]. QCNNs have the potential to surpass classical CNNs in handling certain types of data, such as quantum data or data with inherent quantum properties [15]. This opens up possibilities for applications in quantum-enhanced machine learning, where traditional computing models may fall short. Our focus is the single band Fermi-Hubbard model. Our interest is motivated by the fact that, despite its simplicity, this model captures a lot of aspects of the complex physics of many-body systems. We focus on 1D at first and successively 2D spin lattices, whose complete characterization of the phase diagram remains an open problem. As a test-case, we first investigated 1D Hubbard chains reproducing with our quantum algorithm the signature of a charge gap at half-filling, which persists with increasing system sizes, confirming the preservation of the Mott insulator phase. The quantum calculations were validated using exact diagonalization and density matrix renormalization group (DMRG) approaches. In addition, using QCNNs we successfully performed a first, promising phase classification over the metal-insulator phase transition of a 1D chain when varying coupling strength and next-nearest parameter (Fig. 2).

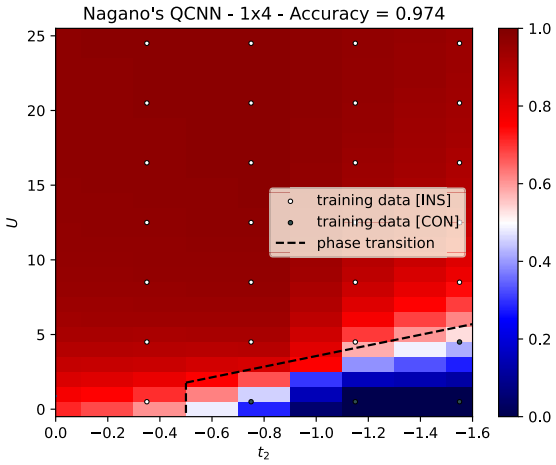

Figure 2: *U vs t_2 phase diagram predictions for the quantum states of a 1×4 lattice. Black points: training set, color: reconstructed pounts.*

In the next steps, we will implement a fully functioning quantum machine learning pipeline that allows for the direct utilization of the system's wavefunction rather than solely relying on its observables, eventually extending our study to 2D materials for which a large curated database exists within MARVEL. An ambitious way to reach our goal would be the implementation of a tensor network-inspired QCNN structure, exploiting its intrinsic capabilities for an enhanced understanding and classification of quantum phases.

g) *Quantum dynamics of magnetic material* Simultaneously, quantum simulations have recently emerged as a powerful tool for scientific research, providing a unique avenue to explore complex quantum systems. One notable project focuses on simulating the Heisenberg model, driven by its broad relevance in fields such as condensed matter physics and quantum information science. The project specifically emphasizes the optimization of trotterized Heisenberg circuits, with a particular focus on employing efficient transpilation techniques at the pulse level to make optimal use of the limited coherence times of current noisy quantum hardware. Observable parameters of interest include magnetization, as well as static and dynamical correlations, with the latter serving as a gateway to the study of Green's functions and other dynamic observables [16]. The natural progression involves integrating noise learning and error mitigation techniques, such as probabilistic error cancellation (PEC). The collaborative effort with IBM and Nicola Marzari's group aims at simulating large-scale systems of interest in material science.

2 Contribution to overall goals and initial proposal

The research contributions presented above align with our original proposal. The variational embedding scheme has moved from preliminary calculations on spin systems to the study of molecules, proving that via the addition of classical resources we can improve the accuracy of quantum simulation without increasing circuit width and depth.
The interface between Qiskit Nature and classical electronic structure codes has been enlarged with the addition of CP2K, enabling the simulation of realistic materials that leverage IBM quantum computing accelerators.
As an important update, Zoë Holmes, EPFL faculty, joined the project in 2023. She has one PhD student (Manuel Rudolph) as an affiliate member, and has hired a postdoc (Tyson Jones) who is first visiting for three months from December, and then will join full-time from early summer 2024. She plans on building on recent work on quantum-inspired classical simulation methods [17, 18] to develop new meta-learning algorithms and as well as tools for finding ground states. In both cases she intends on exploring hybrid methods where the classical simulations are enhanced with data obtained from quantum hardware.

3 Collaborative and interdisciplinary components

After the initial phase of this project, several methods have been developed and demonstrated on small problems. An important next step is to move to larger, physically interesting problems. This is especially interesting, as we investigated several hybrid methods that should allow to scale our simulations to larger systems. In order to understand what physical systems that fit the requirements imposed by our methods could be of particular interest, we started interdisciplinary discussions with other MARVEL investigators. In particular, we discussed a potential application of our hybrid real-time dynamics algorithm to quantum impurity models with Philipp Werner. Discussions with Nicola Marzari's group happen also on a regular basis, among all the different groups involved in the project.

MARVEL publications

List of publications either resulting directly from the NCCR (marked with a red hexagon) or with minor contributions from the NCCR.

- [1] 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*, arXiv:2302.04919 (2023).
- [2] S. Barison, F. Vicentini, and G. Carleo, *Embedding Classical Variational Methods in Quantum Circuits*, arXiv:2309.08666 (2023).
- [3] G. Gentinetta, F. Metz, and G. Carleo, *Overhead-constrained circuit knitting for variational quantum dynamics*, arXiv:2309.07857 (2023).
- [4] D. Linteau, S. Barison, N. Lindner, and G. Carleo, *Adaptive projected variational quantum dynamics*, arXiv:2307.03229 (2023).
- [5] L. Nagano, A. Miessen, T. Onodera, I. Tavernelli, F. Tacchino, and K. Terashi, *Quantum data learning for quantum simulations in high-energy physics*, Physical Review Research **5**, 043250 (2023).

Other references

[6] M. Rossmannek, P. K. Barkoutsos, P. J. Ollitrault, and I. Tavernelli, *Quantum HF/DFT-embedding algorithms for electronic structure calculations: Scaling up to complex molecular systems*, The Journal of Chemical Physics **154**, 114105 (2021).

[7] S. Bravyi, G. Smith, and J. A. Smolin, *Trading Classical and Quantum Computational Resources*, Physical Review X **6**, 021043 (2016).

[8] K. Mitarai and K. Fujii, *Constructing a virtual two-qubit gate by sampling single-qubit operations*, New Journal of Physics **23**, 023021 (2021).

[9] K. Mitarai and K. Fujii, *Overhead for simulating a non-local channel with local channels by quasiprobability sampling*, Quantum **5**, 388 (2021).

[10] S. Barison, F. Vicentini, and G. Carleo, *An efficient quantum algorithm for the time evolution of parameterized circuits*, Quantum **5**, 512 (2021).

[11] H. R. Grimsley, S. E. Economou, E. Barnes, and N. J. Mayhall, *An adaptive variational algorithm for exact molecular simulations on a quantum computer*, Nature Communications **10**, 3007 (2019).

[12] G. Carleo and M. Troyer, *Solving the quantum many-body problem with artificial neural networks*, Science **355**, 602 (2017).

[13] J. Stokes, S. De, S. K. Veerapaneni, and G. Carleo, *Continuous-variable neural network quantum states and the quantum rotor model*, Quantum Machine Intelligence **5**, 12 (2021).

[14] I. Cong, S. Choi, and M. D. Lukin, *Quantum convolutional neural networks*, Nature Physics **15**, 1273 (2019).

[15] H.-Y. Huang, M. Broughton, J. Cotler, S. Chen, J. Li, M. Mohseni, H. Neven, R. Babbush, R. Kueng, J. Preskill, and J. R. McClean, *Quantum advantage in learning from experiments*, Science **376**, 1182 (2022).

[16] C. A., F. Tacchino, M. Grossi, P. Santini, I. Tavernelli, D. Gerace, and S. Carretta, *Quantum hardware simulating four-dimensional inelastic neutron scattering*, Nature Physics **15**, 455 (2019).

[17] E. Fontana, M. S. Rudolph, R. Duncan, I. Rungger, and C. Cîrstoiu, *Classical simulations of noisy variational quantum circuits*, arXiv:2306.05400 (2023).

[18] M. S. Rudolph, E. Fontana, Z. Holmes, and L. Cincio, *Classical surrogate simulation of quantum systems with LOWESA*, arXiv:2308.09109 (2023).

List of year 10 publications related to the Quantum Simulation project

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).

○ D. T. Hoang, F. Metz, A. Thomasen, T. D. Anh-Tai, T. Busch, and T. Fogarty
Variational quantum algorithm for ergotropy estimation in quantum many-body batteries
Physical Review Research **6**, 013038 (2024).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.10376853

○ N. Astrakhantsev, G. Mazzola, I. Tavernelli, and G. Carleo
Phenomenological theory of variational quantum ground-state preparation
Physical Review Research **5**, 033225 (2023).
Group(s): Carleo, Tavernelli / Project(s): QS

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

○ G. Gentinetta, D. Sutter, C. Zoufal, B. Fuller, and S. Woerner
Quantum Kernel Alignment with Stochastic Gradient Descent
in *2023 IEEE International Conference on Quantum Computing and Engineering (QCE)* (2023), pp. 256–262.
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.7804477

⬢○ L. Nagano, A. Miessen, T. Onodera, I. Tavernelli, F. Tacchino, and K. Terashi
Quantum data learning for quantum simulations in high-energy physics
Physical Review Research **5**, 043250 (2023).
Group(s): Tavernelli / Project(s): QS

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

⬢○ A. Nykänen, A. Miller, W. Talarico, S. Knecht, A. Kovyrshin, M. Skogh, L. Tornberg, A. Broo, S. Mensa, B. C. B. Symons, E. Sahin, J. Crain, I. Tavernelli, and F. Pavošević
Toward Accurate Post-Born–Oppenheimer Molecular Simulations on Quantum Computers: An Adaptive Variational Eigensolver with Nuclear-Electronic Frozen Natural Orbitals
Journal of Chemical Theory and Computation **19**, 9269 (2023).
Group(s): Tavernelli / Project(s): QS

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

⬢○ A. Kovyrshin, M. Skogh, A. Broo, S. Mensa, E. Satin, J. Crain, and I. Tavernelli
A quantum computing implementation of nuclear-electronic orbital (NEO) theory: Toward an exact pre-Born–Oppenheimer formulation of molecular quantum systems
The Journal of Chemical Physics **158**, 214119 (2023).
Group(s): Tavernelli / Project(s): QS

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

⬢○ F. Pavošević, I. Tavernelli, and A. Rubio
Spin-Flip Unitary Coupled Cluster Method: Toward Accurate Description of Strong Electron Correlation on Quantum Computers
The Journal of Physical Chemistry Letters **14**, 7876 (2023).
Group(s): Tavernelli / Project(s): QS

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

⬢○ M. John, J. Schuhmacher, P. Barkoutsos, I. Tavernelli, and F. Tacchino
Optimizing Quantum Classification Algorithms on Classical Benchmark Datasets
Entropy **25**, 860 (2023).
Group(s): Tavernelli / Project(s): QS

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

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

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

⬢○ D. J. Egger, C. Capecci, B. Pokharel, P. K. Barkoutsos, L. E. Fischer, L. Guidoni, and I. Tavernelli
Pulse variational quantum eigensolver on cross-resonance-based hardware

Physical Review Research **5**, 033159 (2023).
Group(s): Tavernelli / Project(s): QS

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

A. Kovyrshin, M. Skogh, L. Tornberg, A. Broo, S. Mensa, E. Sahin, B. C. B. Symons, J. Crain, and I. Tavernelli
Nonadiabatic Nuclear–Electron Dynamics: A Quantum Computing Approach
The Journal of Physical Chemistry Letters **14**, 7065 (2023).
Group(s): Tavernelli / Project(s): QS

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

G. Gentinetta, F. Metz, and G. Carleo
Overhead-constrained circuit knitting for variational quantum dynamics
arXiv:2309.07857 (2023).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: github.com/gentinettagian/circuit-cutting-pvqd

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
arXiv:2302.04919 (2023).
Group(s): Carleo / Project(s): QS

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

S. Barison, F. Vicentini, and G. Carleo
Embedding Classical Variational Methods in Quantum Circuits
arXiv:2309.08666 (2023).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: github.com/StefanoBarison/hybrid_ansatz

D. Linteau, S. Barison, N. Lindner, and G. Carleo
Adaptive projected variational quantum dynamics
arXiv:2307.03229 (2023).
Group(s): Carleo / Project(s): QS

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

I. Nha Minh Le, O. Kiss, J. Schuhmacher, I. Tavernelli, and F. Tacchino
Symmetry-invariant quantum machine learning force fields
arXiv:2311.11362 (2023).
Group(s): Tavernelli / Project(s): QS

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

W. Dobrautz, I. O. Sokolov, K. Liao, P. López Ríos, M. Rahm, A. Alavi, and I. Tavernelli
Ab Initio Transcorrelated Method enabling accurate Quantum Chemistry on near-term Quantum Hardware
arXiv:2303.02007 (2023).
Group(s): Tavernelli / Project(s): QS

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

4.3 List of new projects

Lyndon Emsley

Lyndon Emsley, who has already contributed to the NCCR in the previous phases by pioneering the application of machine-learning models to solid-state nuclear magnetic resonance, joined Pillar 2 in year 10 to provide direct application to experimental problems of its infrastructural and methodological developments. In particular, Jacob Holmes, postdoc in his group, will use predictions of the chemical shieldings obtained by improved versions of the shiftML model to further increase the resolving power of NMR crystallography.

Zoë Holmes

Zoë Holmes joined MARVEL in the Quantum Simulations project in 2023. She now has two PhD students (Manuel Rudolph, Joe Gibbs) as affiliate members, and has hired a post doc (Tyson Jones) who will first visit for three months from December, and then join full-time from early summer next year. She plans on building on recent work on quantum-inspired classical simulation methods to develop new meta-learning algorithms and as well as tools for finding ground states. In both cases she intends on exploring hybrid methods where the classical simulations are enhanced with data obtained from quantum hardware.

Michael Herbst

In May 2023 Michael Herbst joined MARVEL as a PI in Pillar 3. His research focus is the understanding of simulation errors in density-functional theory with the aim to improve the reliability of materials simulations. In this direction his prior work includes novel density-functional theory (DFT) algorithms, which automatically adapt the numerics to the physics of the simulated material. Within Pillar 3 he and his team will work on integrating their density-functional toolkit (DFTK) — a DFT code tailored to mathematical research — within the MARVEL software ecosystem to provide a unique platform for prototyping and validating novel algorithms directly in the high-throughput regime.

Associated PIs from PSI

At PSI, Laura Grigori (head of Laboratory for Simulation and Modelling) and Matthias Krack (head of Multiscale Materials Modelling Group) have now become possible hosts for INSPIRE Potentials fellowships.

5 Structure-related aspects

5.1 Education & Training

We keep supporting the growth of students and young scientists in all age groups, from high-school students (from whom we organized a summer camp and information days) to Master students (with new digital education tools that we started to develop this year) to PhDs and postdocs both within and outside MARVEL, to whom we devoted a wide range of activities including a highly successful junior retreat, several international schools and a growing collection of online educational tools.

5.1.1 PhD students and postdocs

In the MARVEL community

Junior seminars and junior retreats

We are continuing to encourage junior scientists to take the lead on events stimulating interactions and collaborations between different groups and institutions. In this line, the junior seminars were relaunched in a hybrid mode in 2023, after an interruption due to the buildup of the Psi-k 2022 conference. With a similar goal, the junior retreats were reinstalled following a recommendation of the review panel at the last site visit, with a new edition in September 2023 and again in 2024.

Junior seminars MARVEL junior seminars are a monthly activity which was initially held on campus at EPFL, and was then moved to a virtual format during the pandemic. They aim to intensify interactions between MARVEL junior scientists from different research groups. The MARVEL junior seminar series was rebooted, and since 2023 is in hybrid mode, in order to maintain in-person contacts and allow off-campus attendees to follow the seminars remotely. More details are given in section 5.4 on Communication & Outreach.

Junior retreat Five years after the last edition, the junior scientists of MARVEL got together for the MARVEL junior retreat that took place in Davos on September 11–15. The meeting was organized by four PhD students, Virginie de Mestral in Luisier's group, and Stefano Barison, Gian Gentinetta and Gabriel Pescia from Carleo's group. It gathered almost 60 PhD students and postdocs from the MARVEL-affiliated laboratories across all partner institutions (Fig. 1) and provided the opportunity to network, exchange ideas, start new collaborations and gain important skills for their future careers. The focus of the retreat was "building bridges": not only between different research directions but also between industry and academia. By bringing together ideas and people from the two worlds, the workshop aimed to facilitate discussions, enabling participants to explore the practical applications of research and forge partnerships that bridge theory with real-world impact. The program featured three guest speakers, who shared about their different experiences: Leopold Talirz, a former MARVEL member at EPFL who is now working for Microsoft Quantum; Erich Wimmer, co-founder, Chief Scientific Officer and Chairman of the Board of Materials Design, and head of the MARVEL In-

Figure 1: *Group picture at the MARVEL junior retreat.*

dustrial Advisory Board; Maximilian Amsler, former MARVEL member at UniBas, formerly at Cornell University and now a research scientist at Bosch Corporate Research and Advance Engineering. The rest of the speakers were junior MARVEL members presenting their current research, also including a poster section accompanied with 2-minute pitch presentations. More information can be found in the official retreat website and in the news on the MARVEL website.

Education platform

OSSCAR Open Software Services for Classroom and Research (OSSCAR), www.osscar.org, which provides a platform to develop, deploy, access and share material for teaching and learning in the form of web applications, has been integrated this year in the *Work* section of Materials Cloud, exploiting its infrastructural resources. It is disseminated widely through the CECAM network and beyond. It is a collaborative environment. As an example, Michele Ceriotti bases his Bachelor course on "Introduction to Atomic-scale modeling" on interactive Jupyter notebooks that integrate chemiscope.org widgets, developed in collaboration with the OSSCAR project and CECAM. OSSCAR notebooks are also used in Sara Bonella's course Computational methods in molecular quantum mechanics.

Lhumos The Learning Hub for Modelling and Simulation (Lhumos) platform is a novel educational platform developed to facilitate the upskilling of students, scientists, and industrial users in HPC applications in the material sciences domain. Lhumos development was supported by MARVEL, MaX, CECAM, MultiXscale, and DOME4.0. Targeted at early-career and more advanced scientists, the e-learning platform gathers videos, lectures, codes, tutorials, seminars, and exercises that cover a wide range of subjects including electronic structure calculations, molecular dynamics, high performance computing, and code optimization. A first test version has now been launched (alpha.lhumos.org), and a webinar was held on January 15, 2024 — attracting 130 participants — to present the new portal and showcase its sections and materials. In particular, Lhumos is set to be the successor to Material Cloud *Learn*, and already hosts 95% of its content, gearing up for a seamless migration. More details on this platform can be found in the Pillar 3 section of the Research chapter.

Figure 2: *CECAM-MARVEL Classics in molecular and materials modeling with, from left to right, Angel Rubio, Eberhard Gross and Nicola Marzari.*

CECAM-MARVEL Classics in molecular and materials modeling

In the series of lectures entitled "Classics in molecular and materials modeling", launched by MARVEL and CECAM in 2019, lecturers explain their pioneering contributions in the field of molecular and materials simulations at a level appropriate for second-year Master and graduate students. The lectures are followed by an interview with the presenters: they are asked to recall the period, problems, people and circumstances that accompanied the creation of milestone methods and algorithms that are now routinely used. The events are recorded and made available on the *Learn* platform of Materials Cloud, and from now on the MARVEL space on Lhumos. While the first two events were held on site at EPFL and attracted about 40–50 participants, the following events were conducted entirely online due to the pandemic, and attracted a much larger audience (up to almost 600 unique viewers). We have since kept the online version to maximize viewership, and also held sessions in hybrid mode if the speakers are available to be present on site. Such a hybrid edition was held on September 28, 2023, featuring Eberhard Gross (Hebrew University of Jerusalem) and Angel Rubio (Max Planck Institute for the Structure and Dynamics of Matter) and entitled: "Time-dependent density functional theory: past, present and future" (Fig. 2). It gathered more than 60 participants on site, with about 200 participants online.

Outside MARVEL

Schools

MARVEL PIs and senior reserachers regularly organize and/or lecture to various schools in the domains of MARVEL.

- In July, Bill Curtin has continued to teach a module on the topic of atomistic simulations at the Texas A&M Computational Materials Science Summer School. This summer school attracts 30–50 PhD students and postdocs worldwide each year.
- Iurii Timrov and Nicola Colonna, senior researchers involved in Pillar 4 co-organized the Advanced QUANTUM ESPRESSO school: Hubbard and Koopmans functionals from linear response at the University of Pavia, on August 28 – September 1. It was a success, with 45 participants, out of more than 160 applications. The core objective of this school was to introduce PhD students, postdocs, and junior scientists to the intricacies of advanced exchange-correlation functionals in DFT, specifically tailored for modeling complex materials, including extended Hubbard and Koopmans functionals. The first two days provided participants with a comprehensive foundation in DFT, density functional perturbation theory, and their basic applications, including ground-state calculations and lattice-vibrational properties. The subsequent two days delved deeply into the theoretical underpinnings of Hubbard and Koopmans functionals, the focal point of our event. We also dedicated a half-day to providing our attendees with a primer on automation techniques, centered around the AiiDA platform, for managing computational workflows involving these cutting-edge methods.
- In November, several young researchers from Michele Ceriotti's group co-organized the Machine Learning Interatomic Potential School for Young & Early Career Researchers (MLIP 2023). This school aimed at young and early-career researchers who are interested in using machine learning interatomic potentials (MLIPs) in their research, introducing to the basic scientific techniques of designing, fitting, and validating MLIPs for chemical/material systems, as well as providing a platform to connect users and developers in a community.

Initiatives in Africa

ASESMA school The 7th edition of ASESMA, the African School on Electronics Structure Methods and Applications took place in Kigali (Rwanda) on June 12 to 23, 2023, and featured several speakers from MARVEL (Fig. 3). Held

Figure 3: *Group picture at the ASESMA school in Kigali, June 2023.*

every two years, ASESMA is organized by the Abdus Salam International Centre for Theoretical Physics (ICTP) in Trieste and consists in a series of lectures and hands-on tutorial sessions that aim to introduce young African researchers to the theory of electronic structure and other atomistic simulation methods, with an emphasis on the computational methods for practical calculations. MARVEL has been supporting the initiative since the third edition in 2015, co-sponsoring it and providing lecturers and mentors. Current members Sara Bonella (CECAM deputy director and group leader at EPFL) and Iurii Timrov (from Nicola Marzari's lab at EPFL), were among the speakers, as well as former member Alberto Carta (from Claude Ederer's group at ETH Zurich). Shobhana Narasimhan (Jawaharlal Nehru Centre for Advanced Scientific Research, India), member of the NCCR MARVEL review panel at SNSF, was also present.

Fellowships for ICTP-EAIFR We are discussing MARVEL support to one (out of four) 2-year Master's fellowship (about CHF 8'000 for 2 years) for the ICTP-East African Institute for Fundamental Research (ICTP-EAIFR), located at the University of Rwanda in Kigali, and partner institute of ICTP in Trieste. This would be part of MARVEL planned support to students from underrepresented groups (in this case, certainly regarding country of provenance) and we will give priority to a woman.

ASESMAnet MARVEL initiated the Atomistic Simulations, Electronic Structure, Computational Materials Science and Applications: the African Network (ASESMAnet), with support now from Psi-k, CECAM and MARVEL (12'000 €/year, 4'000 each) matched by another 12'000 €/year by ICTP. This network funds the visits of African researchers to other researchers or research groups in Africa for focused collaboration of two months or more at a time (half of the funding) and supports exchange of scientists between Africa and Europe

for research collaborations and conference participation (half the funding).

Excellence in Africa (EXAF) The Excellence in Africa (EXAF) joint initiative between EPFL and the Mohammed VI Polytechnic University (Morocco) is meant to foster collaboration between Africa-based young professors and EPFL professors on projects addressing African and global challenges. Steve Ndengué, senior lecturer in the condensed matter physics section of ICTP-EAIFR, Kigali, Rwanda, and Nicola Marzari are working on a project called "Embedded exact quantum dynamics for photocatalytic water splitting", meant to improve understanding of the photochemical processes that might be used in applications, such as producing fuel simply from water and sunlight. This project is relying on a regional computational center located in Rwanda, supported by EPFL, to accurately simulate the dynamics of these chemical processes. The initiative is supporting 1 postdoc and 2 PhD students in Kigali and 1 PhD student at EPFL, namely Marija Stojkovic, under the supervision of Nicola Marzari.

5.1.2 Master students

Courses

Various Master- and PhD-level computational courses are currently offered at participating institutions, taught by MARVEL PIs and other. As an example, Daniele Passerone and Carlo Pignedoli have been teaching for ten years the course "Molecular and Materials Modelling" at ETH Zurich-ITET, where methods of classical and *ab initio* simulation, applied to realistic problems from the research, are introduced to students at the Bachelor and Master level with hands-on sessions based on Jupyter notebooks and access to computational resources inspired by the MARVEL framework.

Advanced modeling online courses

A plan for phase III is to develop structured digital education tools, at the Master level: a library of "advanced modeling courses" including a set of lectures covering different aspects of a modeling technique, completed with lecture notes, self-assessment exercises and (where possible) practical tutorials using actual research software. A first MOOC "Path Integral Methods in Atomistic Simulations" prepared by Michele Ceriotti, has been released and is accessible online[1]. The lecture provides an introduction to path integral techniques applied to the modeling of molecules and materials. It covers molecular dynamics and sampling, the basics of path integrals, advanced path integral methods, ring-polymer molecular dynamics, and colored-noise methods. It was used for a CECAM school entitled "Path Integral Quantum Mechanics" which took place on June 4–8. Participants with little experience with path integral methods and/or i-PI were invited to prepare for the advanced school by following the MOOC before the start of the school. About 60 people participated, and were very positive about the experience. More generally, the homepage of the MOOC has been accessed more than 3'000 times

[1] https://tinyurl.com/pimd-mooc

5.1.3 For the younger generation

MARVEL high-school summer camp

This year's MARVEL summer camp *Des atomes aux ordinateurs, à la découverte de la programmation scientifique*, organized in collaboration with the EPFL Education Outreach Department, took place on June 26–30 and attracted 22 high school students — 10 women and 12 men — for a full week of lectures, exercises and lab visits built around the theme of scientific programming and atomistic modeling. Like in the previous years, the first two days were devolved to a basic introduction to Python, thanks to the expertise of Nicolas Richart and Emmanuel Lanti, two collaborators of SCITAS (Scientific IT & Application Support) at EPFL. Advanced exercises were also planned for more expert students. The next three days took the students through applied exercises in cellular automaton, molecular dynamics and machine learning, thanks to a team of six volunteer PhD students and postdocs from the groups of Michele Ceriotti, Nicola Marzari and Clémence Corminboeuf. The week was enhanced by visits to the clusters of SCITAS and the Swiss Plasma Center, as well as a guided tour of the EPFL campus (Fig. 4, left and center). Student evaluations indicated that the week was a success. Student enjoyed discovering EPFL, making friends, the availability and patience of the teachers. Although some found the exercises sometimes too difficult, they noted that with some help they could manage to solve them. Half the students were from Switzerland (from the French speaking part, as well as one from Zurich) and the other half were from different countries in Europe (BE, IT, ES, RO, CZ), as well as Turkey and USA.

Figure 4: *Left and center: MARVEL summer camp* Des atomes aux ordinateurs, à la découverte de la programmation scientifique *on June 26–30, 2023. Right: Lab visit during the EPFL information days for high school students on November 23, 2023.*

The summer camp was spearheaded by Michele Ceriotti, who as high-schooler took part in something similar at CSCS that inspired him to choose a career in simulation, and is now coordinating its content. A new edition is being planned for June 24–28, 2024.

With the support of the review panel as stated in their report after the 2023 site visit, we are currently looking at the possibility for participating PhD students to get teaching credits for their involvement in teaching this summer camp. Rules are different from a department to another at EPFL, thus we may have to deal case by case. A request to the doctoral school in Materials has been put forward.

Other activities

EPFL information days for high school students

The EPFL information days for high school students are an opportunity to educate high school students on research domains through presentations and demonstrations. On November 24, Anirudh Raju Natarajan and Michael Herbst participated with a common presentation describing the use of computational materials in designing high-performance materials, welcoming three groups of about 20 students. On the day before, the Marzari group welcomed six groups of 6–12 high school students. This took the form of a "lab-visit" given by a 100% female team. Under the supervision of the scientific manager, a PhD student and a postdoc presented their research accompanied with hands-on experiments on phonons and practical activities using the Interactive phonon visualizer available on the *Work* section of Materials Cloud (Fig. 4, right).

5.2 Knowledge & Technology Transfer

Materials Cloud and the AiiDAlab workflow frontend remain at the core of our knowledge transfer efforts, allowing us to share the results of our work with a wider research community that keeps growing. In parallel, in year 10, we leveraged international (e.g. BIG-MAP) and national (SwissTwins) collaborations and conferences (e.g. PASC23) to reinforce ties with the community, and we devoted the 20203 MARVEL junior retreat to technology transfer and academic/industry collaborations.

5.2.1 Knowledge transfer

Software

Materials Cloud

Materials Cloud is central to MARVEL. It is built to enable the seamless sharing and dissemination of resources in computational materials science, offering educational, research, and archiving tools; simulation software and services; and curated and raw data. All its sections (*Learn*, *Work*, *Discover*, *Explore*, *Archive*) are continuously populated and more details on the new features can be found in the Pillar 3 section of the Research chapter. The Materials Cloud *Archive* is officially recommended by the SNSF as a repository to deposit materials-science data, as well as by *Nature*'s *Scientific Data* and the European Commission's *Open Research Europe*.

Most year 10 efforts focus on consolidation toward sustainability beyond the end of MAR-

VEL, as it can be seen from the ongoing migration of the JavaScript backend to the modern React framework, the migration of the Materials Cloud *Archive* to the upcoming InvenioRDM v12 release (scheduled in spring 2024), and the development of Lhumos to replace the *Learn* section. Moreover, new sections offering curated data have been published (fully updated MC3D database, and the section on verification of DFT codes), and the *Archive* has been tightly integrated with the OPTIMADE API by providing a new service that can convert entries with crystal structure files into a fuslly fledged OPTIMADE REST API server.

AiiDAlab and Quantum Mobile

The AiiDAlab web platform gives users access to their personal AiiDA environment in the cloud, where they can run and manage workflows through tailored and lightweight web applications in the browser. As discussed in detail in the Pillar 3 section, in addition to significant platform improvements (robustness, testing, speed), the AiiDAlab QUANTUM ESPRESSO app has been significantly extended with a plugin interface to provide easily new computational capabilities, and with detailed user documentation.
Quantum Mobile, a virtual machine for computational materials science, has become a model for knowledge transfer in real and virtual training events. Standard, but modular and customizable, virtual machines have been used in over 10 tutorials and events, with very good testimonials. In year 10 we have been focusing on releasing a version of Quantum Mobile customized for the QUANTUM ESPRESSO app, to make the startup of the app extremely fast. In addition, a version working also on the new Apple M1/M2/M3 chips has been made available.

AiiDA

AiiDA 2.3, 2.4 and 2.5 were released in year 10, and the developments and improvements are presented in the Pillar 3 section. Beside the code development, one major activity is its dissemination through the scientific community and beyond. In particular, AiiDA was introduced end of August at the Advanced QUANTUM ESPRESSO school in Pavia, along with a short tutorial and examples of recent development in workflows that automatically apply Hubbard corrections. The AiiDA user support has been consolidated in a single new Discourse channel. Since its creation in July 2023, already over 400 posts have been created, showing active engagement and use of AiiDA in the community.

New releases, open source codes

In year 10, several new open source codes were released, with, e.g.,

- Metatensor[2], a specialized data storage format for all your atomistic machine learning needs and more (Ceriotti group);
- DFTK, the density-functional toolkit[3], a library of Julia routines for interdisciplinary research on plane-wave density-functional theory (DFT) algorithms (Herbst group);
- NetKet[4], the machine-learning toolbox for quantum physics (Carleo group);
- qtpyt[5], a quantum transport library based on the non equilibrium Green's function (NEGF) formalism written in Python (Passerone group);
- a new release of chemiscope[6] including visualization of scalar and vectorial atomic properties;
- SPA^{H}M[7], for the generation of local and global representations of spectrum of approximated Hamiltonian matrices (Corminboeuf group).

Generally, open source codes developed by MARVEL researchers are listed on the MARVEL website.
To support the use of these codes, tutorials were organized by the developers, in particular a webinar entitled "Julia for Materials Modelling" was organized by Michael Herbst on May 24, providing a short overview of the current state the code in the multidisciplinary field of atomistic materials modeling and perspectives for using it in this field. Its recording is available in the *Learn* section of the Materials Cloud platform in the MARVEL seminars and tutorials section.

Collaborations and other conferences

European synergies

BIG-MAP Thanks to collaborations with the European BIG-MAP project, an AiiDA + AiIDAlab interface has been developed (and is currently used in production for research) to

[2] https://lab-cosmo.github.io/metatensor/latest/
[3] https://docs.dftk.org/stable/
[4] https://www.netket.org/
[5] https://pypi.org/project/qtpyt/
[6] https://chemiscope.org/
[7] https://github.com/lcmd-epfl/SPAHM-RHO

Figure 5: *"BIG-MAP EUnified Battery Data Space workshop", Grindelwald, January 29–31, 2024.*

drive robotic experiments to assemble and test battery cells, in collaboration with Prof. Corsin Battaglia's lab at Empa. In addition, the development of the next generation of the Materials Cloud *Archive* benefits from the collaboration with BIG-MAP (that has deployed a private version of an Archive, inspired by the public one, to securely share data within the project).

The "BIG-MAP EUnified Battery Data Space workshop" took place on January 29–31, 2024, in Grindelwald. Participants were invited by the organizers Nicola Marzari (EPFL), Giovanni Pizzi (PSI), Tejs Vegge (DTU), and Ivano Castelli (DTU). All representatives of the various Battery2030+ projects — both senior and junior researchers. In total, the meeting hosted 49 participants (Fig. 5). Since the field carries significant overlap with MARVEL areas of research, several MARVEL members joined the event and the logistics was facilitated by the MARVEL program manager.

2D-PRINTABLE Nicola Marzari is part of the 2D-PRINTABLE EU-project aiming at developing new 2D materials and heterostructures for printed digital devices, which started in October 2023. His contribution will build on the Materials Cloud two-dimensional crystals database (MC2D)[8], resulting from high-throughput computational exfoliation of 3D crystal structures, flagship work within MARVEL.

Other collaborations MARVEL continues benefiting from collaborations and cooperations with several European initiatives, e.g., the core partnership with H2020 MaX, NEP, DOME 4.0, or OpenModel.

[8] https://www.materialscloud.org/discover/mc2d/

Other Swiss synergies

Significant collaborations are ongoing with the SwissTwins project, a Swiss replacement to the EuroHPC calls, with direct funding from SERI and coordinated by CSCS. SwissTwins provides support to AiiDA core developments, as well as focusing on direct support for the new interfaces on the Alps infrastructure (FirecREST API, Sarus containerisation).
Tight collaborations are also ongoing with the ORD Establish project PREMISE, aiming at streamlining the exchange of data between AiiDA and electronic lab notebooks (ELNs) toward seamless FAIR data both for simulations and experiments.
Further adoption of AiiDA also beyond materials science is happening in collaboration with the ORD Explore project led by Dr. Stephan Henne at Empa, using AiiDA for Regional Inverse modeling of greenhouse gases.

Conferences organized by MARVEL members

As every years, MARVEL members organized or co-organized conferences, tutorials or workshops, with at least 14 in year 10, and some were also sponsored by MARVEL. All are listed in the NIRA database and on the website (nccr-marvel.ch/ctw). A selection is given here.

- MARVEL sponsored the PASC23 conference which took place in Davos on June 26–28. Among the community, Joost VandeVondele co-organized a mini-symposium about "High performance and high throughput approaches in material science simulations: a European perspective" and Michael Herbst one about "Interdisciplinary challenges in multiscale materials modelling". Four MARVEL PIs (Sara Bonella, Nicola Marzari, Giovanni Pizzi, and Carlo Pignedoli) had invited talks and several posters were prepared by MARVEL members.
- Michele Ceriotti organized with Cecilia Clementi, Gabor Csanyi, and Lixin Sun, the CECAM-Psi-k Conference "Bridging length scales with machine learning: from wavefunctions to thermodynamics" on June 19–23 at Freie Universität Berlin in Germany with more than 150 participants (Fig. 6), benefiting of MARVEL sponsorship.
- As every year since 2019, Giovanni Pizzi has been co-organizing the Open Databases Integration for Materials Design (OPTIMADE) conference, which took place on June 5–9 at CECAM EPFL. Next

Figure 6: *CECAM-Psi-k Research Conference "Bridging length scales with machine learning: from wavefunctions to thermodynamics", Berlin, June 19–23, 2023. More pictures on the website.*

edition will be also at CECAM EPFL on June 10–14, 2024.

Other seminars of interest to the MARVEL community

- On May 25, a seminar jointly hosted by MARVEL and the EPFL Physical Chemistry Seminars featured Vojtech Vlcek (University of California Santa Barbara) addressed the topic "Excitations dynamics driving electronic correlations in molecules and solids".
- On June 2, Zhiting Tian, associate professor at Cornell University, presented a seminar dedicated to thermal phonon transport for energy applications.
- On June 16, a seminar jointly hosted by MARVEL and EPFL's Centre for Quantum Science and Engineering (QSE) featured Andrew Briggs, Professor of Nanomaterials at the University of Oxford, who gave a presentation entitled "Accelerating quantum technologies with machine learning".

5.2.2 Technology transfer

Raising awareness of technology transfer among junior researchers

Leading topic at the MARVEL junior retreat

The theme of the 2023 edition of the MARVEL junior retreat was "Building bridges": between different research lines, but most of all between industry and academia. By bringing together ideas and people from the two worlds, the workshop aimed to facilitate discussions, enabling participants to explore the practical applications of research and forge partnerships that bridge theory with real-world impact. The participants were also invited to take part in a poster competition, where the ultimate stage consisted of marketing their research to non-specialists in an elevator pitch-format, with a strong focus on storytelling.

An initiative to revive the NCCR MARVEL Members and Alumni LinkedIn private group was proposed at the term of the retreat, with the goals of strengthening, expanding, and perpetuating collaborations and technology transfer during and beyond the MARVEL project (more details in the Social media section p. 72).

Round table at the Review and Retreat

During the last Review and Retreat in January 2024 in Grindelwald, a 45-minute round table took place on industrial careers and technology transfer with the MARVEL Industrial Advisory Board. Moderated by Bill Curtin, Erich Wimmer (Materials Design), Nicolas Cudré-Mauroux (SICPA) and Arnaud Grandeury (Novartis) shared with the MARVEL members their visions and advice on how to enter the world of industry from the academic world. We have heard about networking, spark in the eyes, not failing without learning, etc. "Science is only about curiosity, research is finding solutions, innovation is about creating value" said Nicolas Cudré-Mauroux.

From MARVEL to industry — Interviews on the website

Many former members have moved to the industry after working as PhD students or postdocs in one of the MARVEL laboratories. From ICT to energy, from chemical engineering to automotive, several industry sectors value the skills and competences that can be developed doing research on computational materials science. In this new section of the website, we talk to some former MARVEL members who are now working in the private sector, to know more about their experience and the advice they have for younger researchers who are interested in careers beyond academia. The first interviews draw up portraits (Fig. 7) of

- Leopold Talirz, formerly with Berend Smit's laboratory at EPFL, now Senior

Figure 7: *Four MARVEL former members who have moved to the industry. From left to right, Leopold Talirz, Giulia Mangione, Leonid Kahle and Sandip De.*

Software Engineer in the Azure Quantum team at Microsoft;

- Giulia Mangione, formerly in Clémence Corminboeuf's group at EPFL, now Design Tech Lead at Stellantis;
- Leonid Kahle, former PhD and then postdoc in Nicola Marzari's lab at EPFL, now working for Materials Design Inc, a company specializing in atomistic simulation software;
- Sandip De, postdoc in Michele Ceriotti's lab at EPFL from 2015 to 2018, now leader of a team working on quantum mechanical simulation at BASF.

New interviews will be added regularly.

Other actions

Trainings on IP rights and transfer to industry will be proposed at the 2024 junior retreat.

Industrial Advisory Board

Since the beginning of phase II, an Industrial Advisory Board (IAB) was established, bringing together six representatives of the industrial sectors of interest to MARVEL. Two of these members — Frédéric Diologent (Richemont) and Ryoji Asahi (Toyota Central R&D Labs) — have now left the board. A new member, Paola Gori Giorgi (principal research manager at Microsoft Research AI4Science) has joined existing members Nicolas Cudré-Mauroux (SICPA), Thomas Eckl (Bosch GmbH), Arnaud Grandeury (Novartis), and Erich Wimmer (Materials Design).

Industrial collaborations

Broad collaborations with Solvay, Samsung, or Bosch, are continuing in phase III, and some new ones have started, e.g., with one pharmaceutical company, or an Innosuisse project of Luisier's group with Lumiphase. MARVEL members are also hired by industries, e.g., BASF, Microsoft, or Materials Design.
An ongoing collaboration with BASF is demonstrating the technological impacts of the machine learning developments in Pillar 2 [1].

Industry day at Empa

We are planning to organize this year an Industry day, as a collaboration between Empa and MARVEL, as suggested by the review panel at the last site visit.

Other activities

Anirudh Raju Natarajan gave a seminar as part of the EPFL Engineering Industry Day in March. This event is an opportunity to connect companies with research laboratories to establish new collaborations.

MARVEL publications

[1] N. Lopanitsyna, G. Fraux, M. A. Springer, S. De, and M. Ceriotti, *Modeling high-entropy transition metal alloys with alchemical compression*, Physical Review Materials **7**, 045802 (2023).

5.3 Equal Opportunities

The promotion of gender equality is a major focus for MARVEL. We continue to build on our flagship measures and activities (e.g., the INSPIRE Potentials MARVEL Master's Fellowships, the activities for girls and young women, Agility Plus funding, #NCCRWomen campaign) to strengthen the recognition of women researchers and increase their visibility.

5.3.1 Advancements of women scientists

Leadership of projects & allocation of funding

An amount of 400'000 CHF was allocated in phase III to integrate new junior and women researchers. It was decided to use this funding to support two women PIs, Sara Bonella, already in Pillar 3 since the beginning of the phase, to increase her funding, and Zoë Holmes, in the Quantum Simulation project, as a recently hired assistant professor at EPFL.

INSPIRE Potentials fellowships

New recipients In year 10, through the two calls, we could offer nine new INSPIRE Potentials fellowships, five in April, including an anticipated application in January (plus one additional who declined), and four in October, including a late application in December. To summarize, in addition to Noémie Hu and Eva Doloszeski, who were already selected in 2022 and started in February and September 2023, repectively, we are happy to welcome for 6 months (Fig. 8)

- Jente Clarysse from ETHZ in the group of Mathieu Luisier at ETHZ from end-April 2023,
- Anna Paulish from EPFL in the group of Nicola Marzari at EPFL from August 2023,
- Ayesha Ulde from the Indian Institute of Technology Madras in Chennai in the group of Anirudh Raju Natarajan at EPFL from mid-August 2023,
- Laura Mismetti from EPFL in the group of Ivano Tavernelli at IBM from September 2023,
- Aude Maier from EPFL in the group of Lenka Zdeborová at EPFL from October 2023,
- Serena Bragadini from Università degli Studi di Modena e Reggio Emilia in the group of Nicola Marzari at EPFL from March 2024,
- Valentina Sanella from Università Milano-Bicocca in the group of Nicola Marzari at EPFL from April 2024,
- Hela Mhiri from ENIT, Tunisia and ENSTA, Paris in the group of Zoë Holmes at EPFL from mid-April 2024,
- Jayashree Narayan from the Indian Institute of Science Education and Research Mohali in the group of Sara Bonella at EPFL from August 2024.

Networking event On October 19, a 1.5-hour networking event gathering present and former (now PhD students) INSPIRE potentials fellows was led by the scientific manager with the help of a female postdoc. The idea was to run this session in a spirit of kindness and confidentiality, allowing all the participants to share about their experience or concerns, after a time of exchange by two to learn about each other. The importance of networking was one of the main take-home message. It took place on a Thursday morning, just before a MARVEL junior seminar, enabling those who traveled from out of EPFL to also enjoy to be physically present at the seminar. The initiative was very well appreciate and will be renewed in this or another format.
We also made sure to invite all of them to the MARVEL gathering events, in particular to the junior retreat in September and the Review and Retreat in January.

Good practices for Master's students We do our utmost to ensure that the Master's students feel welcome and that they benefit from a high-quality experience. They have a mentor in the group as a preferential contact person, not only for research but for all questions, helping to join the life in the group and to increase their self-confidence. However, it's not always easy to spot any problems during their stay. At the

Figure 8: *New INSPIRE Potentials students selected in 2023. From left to right, from the April call, Jente Clarysse, Anna Paulish, Ayesha Ulde, Laura Mismetti, Aude Meier, and from the October call, Serena Bragadini, Valentina Sanella, Hela Mhiri, and Jayashree Narayan.*

end of their internship, we are asking them to give some feedback which is kept anonymous. One wrote "I was putting a lot of pressure on myself throughout the internship which resulted in a burn-out at the end of the internship. This was mainly my own doing (I really wanted to achieve something and prove that I was worth the internship), but maybe having clear targets on when to work (so no Slack messages on the weekends) or clear communication on what to achieve would have been good." This kind of feedback is a challenge for us and led to a meeting of a group of women researchers to discuss how we can propose excellence fellowships and at the same time prevent that the recipients put too much pressure of themselves, wanting to show they deserve it, also addressing the impostor syndrome that may arise. As an outcome of this meeting, we plan in the future to also propose a contact outside the group and more informal meetings with present and former INSPIRE Potentials fellows, for example simply for a coffee.

New host groups at PSI With the newly established Laboratory for Materials Simulations at PSI headed by Nicola Marzari, new research groups in computational material science are loosely interacting with MARVEL. Even if they are not directly funded by MARVEL, a suggestion was made to Laura Grigori (head of Laboratory for Simulation and Modelling) and Matthias Krack (head of Multiscale Materials Modelling Group) to be added in the list of labs willing to host INSPIRE Potentials fellows, which they accepted.

Visiting PhD students

At the 2023 site visit, we shared with the review panel our project of setting fellowships for visiting PhD students and junior postdocs from underrepresented groups regarding gender, ethnicity, or any other status, especially women, and researchers from sub-Saharan countries. It appears that the rules, notably at EPFL, make it difficult to set up, with a maximum grant of CHF 2'500 per month, including funding for the student in her or his own country. We are still investigating how to implement these fellowships, or envisioning to set them informally, circulating the possibility among PIs. Also, as mentioned in section 5.1 on Education & Training, we are planing to fund a 2-year Master's fellowship at ICTP-EAIFR in Kigali.

EPFL-WISH Foundation

In 2023, MARVEL decided to contribute once again 5'000 CHF to the EPFL-WISH Foundation fellowships for Masters projects abroad, with the idea of supporting a student in materials science. This was the case of a project focusing on "Perovskite solar cells — Substituting the layer of Indium Tin Oxyde". The EPFL-WISH (Women In Science & Humanitie) Foundation "supports young women in STEM, in particular at EPFL, and encourage them to continue their research and pursue their dreams in a higher professional career" acting on representation, financial support, coaching and recognition of brilliant women across the world.

Career development

MARVEL women researchers were regularly informed about dedicated activities (lunch events, conferences, workshops) organized at EPFL or in other participating institutions, and are encouraged to participate in training, mentoring and coaching programs offered at the various institutions. In particular, in November, a round table for PhD students, organized by NCCR Bio-Inspired Materials, EPFL-WISH foundation, and EPFL Equal Opportunity office, entitled "Planning and advancing your career in industry" and facilitated by Stefania Bellaio, head of R&D Plant Based at Migros, attracted four MARVEL students (from EPFL and ETHZ). It was really appreciated, by its quality and the usefulness and intelligence of the information shared.

5.3.2 Recognition of women researchers' excellence and increase of their visibility

Distinguished lectures and junior seminars

We continuously identify renowned women scientists for the MARVEL distinguished lectures. In year 10, we featured a lecture from Prof. Claudia Felser (MPI CPfS, Dresden), out of the three lectures of the year, and Prof. Elisa Molinari (Univ. Modena and Reggio Emilia) will give the next one in February 2024. Since the beginning of the distinguished lectures series, 13 women and 22 men have participated (i.e., 37% women featured). An effort is also made to feature the diversity of MARVEL in the speakers presenting at the junior seminars, with 5 women and 9 men in the 7 seminars of year 10 (i.e., 36% women featured).

Women of MARVEL

We continue to feed our webpage with portraits of the MARVEL researchers and their testimonies about their triumphs as well as the challenges they face in pursuing their careers, as well as collect testimonials of MARVEL INSPIRE Potentials fellows to promote this tool. Both series were used for the continuation of the #NCCRWomen campaign.

#NCCRWomen campaign

As a continuation of the #NCCRWomen campaign, in 2022–2023 some participating NCCRs decided to feature more women researchers, this time in the form of written portraits and photos on our website and promoted on the campaign's Instagram and Twitter (now X) channels. For Twitter, we can report 673 followers as of January 29, 2024. On the MARVEL side, we drew on the existing portraits that have populated the website since spring 2019, while supplementing our corpus with interviews conducted by Carey Sargent. After a week in November 2022, showcasing our PIs, we were pleased to highlight some MARVEL researchers, Ksenia Briling, Marija Stojkovic, and Giovanna Lani, on February 13–17, and current and former INSPIRE Potentials fellows Melika Honarmand, Linda Mauron, Arianna Cantarella, Yuri Cho, and Virginie de Mestral, on March 27–31 (Fig. 9). The second week was intentionally chosen close to the MARVEL INSPIRE Potentials application deadline of April 15, to enhance the publicity for our fellowships. In March 2023, as part of the #NCCRWomen in school, a "researcher in my class" initiative in 2022–2023, Ksenia Briling (Corminboeuf's group) and Giovanna Lani (Marzari's group) visited a chemistry and a physics classes at Collège Voltaire, a high school in Geneva.
To further build on the #NCCRWomen campaign and take advantage of these videos, we used them as starting points on different occasions, for example for the EPFL Open Days (see p. 73 in section 5.4 on Communcation & Outreach), the lab visits for the girls of the summer camp *Matériaux super géniaux* (see below, section 5.3.3) or during the EPFL information days for high school students (see p. 61 in section 5.1 on Education & Training).

Figure 9: *#NCCRWomen campaign in 2022–2023, with (first line) the portraits of the MARVEL researchers shared on February 13–17 and (second and third lines) the portraits of former and current INSPIRE Potentials fellows shared on March 27–31. Screenshots from Instagram.*

Women's representation in events

We put a lot of attention on women's representation in educational or public events organized by MARVEL or in which MARVEL participates. In particular, in year 10, 4 women (out of 11 researchers) were at the MARVEL stand at the EPFL Open Days, 2 (out of 6) supervised students during the summer camp for high school students, 1 (out of 2) came to help the scientific manager at the lab visit during the summer camp *Matériaux super géniaux*, and a 100% female team hosted the lab visits during the EPFL information days for high school students.

"Women in Materials" artwork and beyond

The "Women in Materials" artwork, presenting female EPFL professors active in the Institute of Materials (IMX), first realized in 2018 based on an idea from Nicola Marzari and sponsored by MARVEL and IMX, was modified in spring 2023 to add the portraits of the recently-appointed Professors Marianne Liebi and Tiffany Abitbol (Fig. 10). In 2019, the project was extended by the EPFL Equal Opportunities Office to "Female Leadership in Science", and portrayed 50 women professors at EPFL on the occasion of EPFL's 50th anniversary. Now, following positive exchanges between our director and Prof. Paul Dyson, dean of the faculty of Basic Sciences at EPFL, they decided to set similar artworks in the entrance halls of the three institutes, Physics, Chemistry and Mathematics. MARVEL will sponsor half the costs and is involved in the realization and the promotion of the project. The practical re-

Figure 10: *The "Women in Materials" artwork, on display in the entry hall of building MX on the EPFL campus..*

alization is currently under study, and the portraits should be visible by summer.

5.3.3 Actions for girls, young women and future scientists

MARVEL continues to support the activities for girls or for girls and boys (with 50% girls) organized by EPFL's Science Outreach Department (Fig. 11). These are always fully booked weeks in advance, with registrations filling up within a few hours/days.
The two editions of the *Polythème* workshop *Diamant, alu, caoutchouc, ils sont fous ces matériaux!* for girls only (one in February with 16 participants and one in November 2023 with 17 participants), took place on three Wednesday afternoons, and enabled participants to discover the extraordinary properties of materials. The next edition will be on February 28, March 6 and 13, 2024. The ninth edition of the summer camp *Matériaux super géniaux*, August 14–18, allowed 20 girls aged 11 to 13 to discover the fascinating world of materials. From discovering polymers to carrying out experiments with crystals, the different families of materials no longer hold any secrets for them. Two lab visits took place during the week, one organized by the MARVEL scientific manager. Making computational research visual for a lab visit is a challenge. Building on activities already developed for different occasions and publics, and making sure the tools and concepts are adapted to their age and knowledge, she built a storytelling showing some research aspects of computational design and discovery of materials, starting with showing two #NCCR-Women portraits of MARVEL scientists, using a 3D crystal-structure visualizer to determine which crystals are 3D and which are 2D and thus maybe exfoliable, playing around with vibrations (sound, heat) to perceive the concept of phonons, and ultimately visualizing those using the Interactive phonon visualizer, this last stage being a huge success. The chemistry summer camp for girls and boys (with 50% girls), August 7–11, with 20 participants, takes place in a real chemistry lab and, with gloves, white coats and protective glasses, the young people wear the same clothes as "real chemists" and discover different aspects of chemistry and its usefulness, doing experiments. The next editions of these two camps will be August 12–16 and 5–9, 2024. respectively.

To this, we can add the continued support of

- the mathematics workshops *Maths en jeu* (with 180 participants in 2023, 101 girls and 79 boys);
- the *Coding club des filles*, offering coding workshops for girls 11 to 15 years old organized throughout French-, German- and Italian-speaking Switzerland.

Moreover, we continue to set aside for girls half of the spots of the MARVEL-organized summer camp for high-school students *Des atomes aux ordinateurs, à la découverte de la programmation scientifique* (see section 5.1.3). Indeed, high-school is a good time to help young women consider university studies in a scientific domain and the summer camp is an opportunity show them a little bit what it looks like.

Figure 11: *Action for girls in 2023. From left to right: Summer camp* Matériaux super géniaux*: MARVEL lab visit and activity during the camp; chemistry summer camp;* Polythème *workshop on materials; mathematics workshops* Maths en jeu*;* Coding club des filles *(© EPFL SPS for all pictures).*

	year 1		year 2		year 3		year 4		year 5		year 6		year 7		year 8		year 9		year 10	
	W	M	W	M	W	M	W	M	W	M	W	M	W	M	W	M	W	M	W	M
Group leaders	4 17%	20 83%	6 18%	27 82%	9 22%	32 78%	8 19%	34 81%	4 13%	27 87%	3 10%	27 90%	7 19%	29 81%	6 19%	26 81%	7 29%	17 71%	5 21%	19 79%
w/o Agil. +																	3 15%	17 85%		
Senior res.	1 13%	7 87%	0 0%	8 100%	2 9%	21 91%	3 10%	28 90%	4 19%	17 81%	3 15%	17 85%	7 27%	19 73%	6 27%	16 73%	3 27%	8 73%	2 22%	7 78%
Postdocs	5 11%	39 89%	8 11%	65 89%	13 16%	69 84%	15 20%	61 80%	13 21%	48 79%	9 16%	49 84%	6 14%	36 86%	7 19%	30 81%	5 16%	26 84%	4 13%	26 87%
PhD	6 26%	17 74%	9 20%	35 80%	9 19%	38 81%	10 19%	43 81%	14 25%	41 75%	18 28%	47 72%	21 35%	39 65%	16 31%	35 69%	20 33%	40 67%	20 34%	39 66%

Table 5.1: *Number and share of women (W) and men (M) involved in MARVEL in years 1 to 10 (From NIRA). In the category "group leaders", in year 10, all people are receiving NCCR funding except Christian Rüegg. Ana Akrap was spending her carryover from phase II until July 2023. In the category "senior researchers", 3 people, 1 women and 2 men, are paid with NCCR funding, at least for part of year 10. In this category, the numbers are too low to be considered on a statistical aspect.*

5.3.4 Work-life balance

All MARVEL members are informed about existing measures such as the SNSF Flexibility grants, day-care facilities and tools for a better work-life balance in the different MARVEL-related institutions, through the website and sharing information in the internal newsletters. Currently, a SNSF Flexibility grant is awarded to a MARVEL member

5.3.5 Numbers

Increasing the proportion of women scientists in STEM fields is a challenge. At the national level, the proportion of women in physics, chemistry, materials science and computer science is very low and MARVEL numbers are at similar levels (Table 5.1).
We worked a lot at the PhD student level to increase the number of women within MARVEL. The main tool has been and still is the INSPIRE Potentials fellowships. This allowed to double the number (and the share) of women PhD students in phase II as compared to phase I. Now, since year 7, we can notice a stabilization of the share of female PhD students a bit above 30% which is rather on the high side compared to what is found in the MARVEL-related domains in Switzerland. At the other levels, the share of women postdocs remains in the low range of previous years, and the total number of senior researchers (9) is too low to be considered on a statistical aspect. Welcoming Zoë Holmes as new PI from year 10 has increased the number of women PIs in the project.

5.4 Communication & Outreach

We continued using a mix of online and in-presence tools to increase the visibility of MARVEL scientists and their results and to communicate to different audiences. In addition to publishing news and scientific highlights on the website and in social media, we organized events such as the distinguished lectures and participated in large events such as the EPFL Open Days. Internal communication was ensured by a variety of tools, including the newsletter, junior seminars and another highly successful Review and Retreat meeting.

5.4.1 Internal and external communication

Website and newsletter

We continued adding to the website (nccr-marvel.ch), contributing to 24 news items on various activities, events, awards and other news of interest to the broader community. We also wrote 16 (as of January 29, 2024) science highlights and feature stories focused on our research. We published 9 internal and scientific newsletters during the year. External readership of the scientific newsletter grew to 563 subscribers, up from 392 in January 2023 and 209 in January 2021.

MARVEL distinguished lectures

MARVEL has organized distinguished lectures given by prominent experts in the fields covered by the NCCR. During 2023, three distinguished lectures were organized, all of them as 50-minute Zoom webinars, which were also recorded and made available on the *Learn* platform of the Materials Cloud and are also available on the MARVEL space of Lhumos.

- Prof. Kristian Sommer Thygesen, from the Technical University of Denmark (DTU), who presented a lecture on "Emergent Properties in Flatland: When One Plus One is More than Two" on March 23.
- Prof. Claudia Felser, from the Max Planck Institute for Chemical Physics of Solids in Dresden (Germany), with a lecture entitled "Chirality and Topology" on May 2.
- Prof. Emmanouil Kioupakis, from the University of Michigan, on "Advancing the state of the art in semiconductor technology through predictive atomistic calculations: from uncovering fundamental limitations to discovering new materials" on June 2.

5.4.2 Internal communication

Review and Retreat

For the second time, the MARVEL Review and Retreat took place in Grindelwald, in the Bern canton, on January 17–19, 2024, involving over 130 people — including PIs, postdocs, PhD students and members of the project's Scientific and Industrial Advisory Boards (Fig. 12). Director Nicola Marzari opened the first day by reminding that the key goal of this third phase of the project is to build a digital infrastructure for materials science and to show the community that it can become a powerful accelerator of research, while keeping pace of a rapidly evolving scenario where machine learning and large language models are changing the rules of the game. Marzari also challenged all groups in the consortium to think critically about the usability and long-term sustainability of open science tools such as the Materials Cloud and AiiDA, on how to make advanced simulation methods available to a larger community, and on the viability of quantum computing for materials science. The sessions were then structured around the main pillars of NCCR MARVEL: on the first day, the sessions on Design and discovery of novel materials, Machine learning for molecules and materials, Digital infrastructure of open simulations and data, Long-term integration in the Swiss scientific landscape were introduced respectively by William Curtin, Michele Ceriotti, Giovanni Pizzi, Nicola Marzari, all of whom were followed by presentations of junior lab members focusing on key results and case studies. The second day was dedicated to the Advanced simulation methods and Quantum simulation projects, introduced by Daniele Passerone and Giuseppe Carleo respectively. The program also included two highly-appreciated opportunities for all MARVEL members to exchange views directly with members of the Industrial Advisory Board (in particular, on the opportunities and challenges of career transitions from academia to industry, see also p. 64 in section 5.2 on Knowledge & Technology Transfer) and of the Scientific Advisory Board.

Figure 12: *MARVEL Review and Retreat in Grindelwald, January 17–19, 2024.*

MARVEL junior seminars

MARVEL has been organizing junior seminars in order to strengthen interactions between the MARVEL junior scientists belonging to different research groups (i.e. PhD and postdocs, either directly funded by the NCCR, or as a matching contribution). Each seminar consists of two 25-minute presentations, followed by time for discussion. During year 10, 7 seminars were organized in hybrid mode, in order to maintain in-person contacts and allow off-campus attendees to follow the seminars remotely. Overall, 14 researchers (representing EPFL, ETH Zurich, PSI, Empa, UniFR) presented their research.

Other meetings

Projects meetings

In order to ensure a continuing and broad research stream between groups, we have striven to ensure that all project teams meet at least four times a year, including the Review and Retreat and the SNSF site visits. With the Review and Retreat in January and the site visit in March/April, we have therefore planned to arrange two online meetings for each project, one in September/October and another in June/July. Project leaders are left free to set up the program for their project meeting (formal structured presentations, general discussions, etc.). The only expectation is that they are sessions of 2-3 hours taking place around the dates mentioned above. All MARVEL members are expected to attend the meetings of the project to which they are affiliated. The project meetings are then announced to all MARVEL members, and everyone is welcome to attend the meetings of other projects. A series of online meetings, one per project, has taken place between September and October 2023.

MARVEL communication open mic session

With SNSF expecting a clear communication strategy and implementation — including giving maximum visibility to the work produced within MARVEL — the NCCR has organized an open mic session to introduce the new communication officer, Nicola Nosengo, who is overseeing all these aspects, organizing news coverage, managing social networks and writing highlights and feature stories about the NCCR's research actuality. The open-mic session allowed MARVEL members to be informed about the editorial schedule and the way news coverage is planned and prepared; to discuss upcoming studies, events and activities that would be suitable for coverage; to raise any issue or relevance for communication. We also took the opportunity to remind attendees how open access in data and publications work.

5.4.3 External communication

Communicating MARVEL research

EurekAlert

We continued using EurekAlert to communicate research results to scientific journalists, publishing 5 press releases on topics deemed to be of interest to the wider scientific and journalistic communities, in line with our strategy of increased outreach to these groups. All releases were viewed more than 200 times according to EurekAlert statistics, and were picked up and relaunched by science journalism websites such as Phys.org.

Social media

X (formerly named Twitter) remains the main focus of our social media work and the account @nccr_marvel has 2'167 followers as of January 25, 2024. We posted an average of more than one Tweet per week over the period, earning over 80'000 impressions (the total sum of all the times a Tweet has been seen) and an average engagement rate (calculated as the total number of engagements such as clicks, retweets, replies, follows or likes that a Tweet receives divided by the total number of views) of 3.5%. On LinkedIn, we have both a MARVEL page, with 471 followers as of January 24, 2024, where we regularly post news, and a LinkedIn private group (NCCR MARVEL Members and Alumni), primarily with the intention of building and reinforcing ties within the MARVEL community and keep contacts with researchers and students who have moved on. This latter was reinforced in year 10, with the idea of building a platform of exchange between former and present MARVEL members, advertising for example job offers. After publicity made in the newsletters and especially at the last Review and Retreat, the group counts 96 members, as of January 29, 2024.

MARVEL in web news and in the press

In addition to the several stories published on the MARVEL website and on the websites of home institutions, MARVEL research results have often been covered by the scientific media. For example, the story on "Solids that are also liquid" on research from Nicola Marzari's group (January 2023) and the story on Ana Akrap's discovery that a material considered a semi-metal is indeed a semiconductor (November 2023), were both featured in Phys.org; a story on Nicola Marzari's group research into a computational model of thermoelectric conversion led to a story on the EPFL website and to one on TechExplore. The story on the massive verification effort of computer codes led by Giovanni Pizzi (November 2023) was featured both in Phys.org and in AZOmaterials.

Events

CECAM-MARVEL Mary Ann Mansigh conversation series

The CECAM-MARVEL "Mary Ann Mansigh conversations", named after Mary Ann Mansigh Karlsen, an outstanding representative of the first generation of coders, whom we had welcomed to EPFL in 2017, focus of non-strictly technical topics of cultural interest for the simulation and modeling community. The format reflects the informative and informal nature of these sessions, with talks introducing the subject followed by a conversation between the speakers and the audience. A fourth conversation, this time on scientific writing and scientific publishing, is planned on April 23, 2024. The two speakers will be Mark Peplow, formerly news editor of *Chemistry World* and *Nature* and now a freelance science journalist who frequently covers chemistry and materials science, and Nina Meinzer, Senior Editor at *Nature Physics*.

EPFL Open Days

On April 29–30, MARVEL participated in the traditional EPFL Open Days, which allowed thousands of visitors to discover the school through events, animations, meetings, workshops and many other initiatives. MARVEL's stand proposed 3D movies and experiments to show how novel materials are created by computational design, explaining magnons and phonons, playing with magnets and compasses on one side, and with sound vibrations and propagation of heat on the other side, and showing how supercomputers are used to build materials properties (Figs. 13 and 14).
Building on the #NCCRWomen campaign, MARVEL invited the other NCCRs present at EPFL to join a part of the stand dedicated to women in science. Visitors could thus meet women researchers from NCCRs SPIN, Automation, Digital Fabrication and MARVEL, discover the #NCCRWomen campaign movies of the four NCCRs, take postcards of the portraits of the "Female Leadership in Science" exhibition, and children could enjoy the colorings from the #NCCRWomen campaign (Fig. 15). They could also read (and take with them) the comics *Cherchez, les femmes!* which was produced by CECAM to show young girls and everyone else that computer simulation and programming is a fun field and can lead to great adventures, and translated to French with the support of MARVEL. All these initiatives wanted to show that we should never let anyone tell us what we can or can't do or study. Neither our gender, nor our origin, nor anything else should be a brake on our choices.
Together with CECAM, two round tables on "Comics & Science" were also organized, with a scientist (Sara Bonella, MARVEL and CECAM), a local cartoonist (Laurent Schafer) and an expert on scientific dissemination (Antonella Del Rosso, CERN) exploring how comics can be used as a tool for scientific dissemination.

Figure 14: *EPFL Open Days on April 29–30, 2023. MARVEL stand. Hands-on experiments on magnons (left) and phonons (right).*

Ig Nobel Award Tour Show

On Tuesday April 16, 2024, after a 5-year break, EPFL will welcome for the fifth time the Ig No-

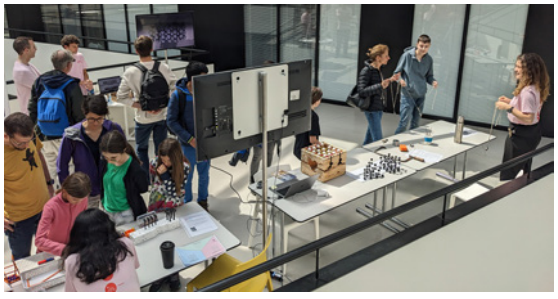

Figure 13: *EPFL Open Days on April 29–30, 2023. MARVEL stand with 3D movies and hands-on experiments on phonons and magnons.*

Figure 15: *EPFL Open Days on April 29–30, 2023. Women in science stand.*

bel Award Tour Show, with Marc Abrahams and a line-up of Ig Nobel Prize winners, with the support of the MARVEL.

NCCR gathering at EPFL

NCCRs MARVEL and Automation organized a NCCR gathering at EPFL on December 4. It started with a discussion time, addressing questions such as making sure that our labs are diversity-friendly environments, sharing on best practices, brainstorming on new collaborative projects between NCCRs. About 25 participants could then extend the discussion over a standing lunch and then visit of the current exhibition at Archizoom. Exchanges between NCCRs are opportunities for rich outcomes.

5.5 Open Science

The Materials Cloud *Archive* has grown into an important open science repository not only for MARVEL but for the whole community, recommended by the European Commission and the SNSF. Our varied open science efforts also include meetings on open data with the other NCCRs and a continuous work to inform and sensitize our scientists on open access requirements.

5.5.1 Introduction

Open Science is central to MARVEL and part of its backbone. In particular, at the research level, Pillar 3 works toward the delivery of a self-sustaining long-term digital infrastructure of open simulations and data.
The MARVEL data manager is the scientific manager, Lidia Favre-Quattropani, and she is supported by the MARVEL data team, with in principle at least one representative per project, available to address questions regarding open research data policy within MARVEL. The role involves being the point of contact in the group, project or institution, and serves to ensure that information is flowing well and easily; to raise awareness of data management; and to check the minimal requirements presented in the MARVEL research data strategy.
MARVEL members are regularly reminded of important pointers related to open access (data and publications) , in particular at the open-mic event and very recently at the Review and Retreat in Grindelwald. The requirements regarding open access are included in each internal newsletter with links on the two dedicated web-pages on open access publications and open research data, also accessible through the MARVEL toolbox at nccr-marvel.ch/toolbox.

Figure 16: *Nicola Marzari (left), with Leopold Talirz and Giovanni Pizzi, former members of his lab and now respectively at Microsoft and PSI, at the National ORD prize ceremony on December 6, 2023.*

5.5.2 Open data

National Prize for Open Research Data

Nicola Marzari and his team at EPFL and PSI received a special acknowledgment from the jury of the National Prize for Open Research Data (ORD Prize), awarded by the Swiss Academies of Arts and Sciences on December 6 (Fig. 16). The theme of the prize was "The re-use of research data", for projects that either re-use data from other projects or make their own data available in such a way that other researchers can conduct further work with it. A detailed news can be read on the MARVEL website.

Joint-NCCRs ORD meetings

A group of NCCRs, led by NCCR Microbiomes and including NCCR MARVEL, have received funding from SNSF, through the NCCR Network Ventures to organize three one-day meetings on Open Research Data (ORD), in Zurich, Lausanne and Basel. The MARVEL scientific manager, in her data officer role, took some time in this project in the spring 2023. MARVEL was heavily involved in organizing the event in Lausanne (Fig. 17). In addition, several of its researchers made plenary presentations: Marnik Bercx and Chris Sewell with a talk entitled "Towards fully reproducible

Figure 17: *Meeting on Open Research Data (ORD) in Lausanne on May 8, 2023.*

workflows with the AiiDA informatics infrastructure", in Lausanne, and Giovanni Pizzi on "Open-research data repositories and reproducible workflow" to showcase the open-science approach and platforms of MARVEL, in Basel.
In preparation for the meeting, a survey was sent to MARVEL researchers (and those of other NCCRs as well) to get their input on a series of topics to ensure that the meetings would meet their needs and interests.
A detailed report was sent by Kendra Brown (NCCR Microbiomes) to the SNSF already in June 2023.

Datasets on Materials Cloud

The Materials Cloud *Archive* has been developed by MARVEL and has become an open repository for research data that has been recommended by entities including the EU Commission and the SNSF, or *Nature*'s *Scientific Data*. The platform receives about 2'500 visitors per month. The moderation of records submitted to the platform is managed by MARVEL program manager Patrick Mayor, who also consults with the technical team on improvements, coordinating with the web engineer. In 2023, 199 records have been published on the Materials Cloud *Archive*.
For MARVEL researchers, the data underlying publications must be submitted to the Materials Cloud *Archive* at the latest at the same time as publication, with no additional costs for the groups. Hosting files on the Materials Cloud *Archive* is a requirement of the funding agencies, and this also makes the data citable (with DOI), ensures long-term preservation of the data for 10+ years, boosts visibility of the research, and increases the citation count. The use of the Materials Cloud *Archive* as an open repository is broadly adopted by MARVEL members. Moreover, for entries already on the Materials Cloud *Archive* by mid-November, we can generate the bibliography files with the related publications, asking the PIs to complete their file with the missing publications (i.e. publications with no dataset deposited on Materials Cloud or publications for which the datasets have been published between November and January).
MARVEL publications in 2023 generated 59 MARVEL-related entries on the Materials Cloud *Archive* as well as 18 entries on other open repositories. The MARVEL dataset index is available on the website, updated every year in February/March. One challenge for the data manager is to track, for each MARVEL publication with no indication about datasets, whether datasets exist, are already deposited somewhere and, if not, ask the authors to do so or why they don't. Finally, it should be noted that for newly submitted publications for which the preprint is available on arXiv.org or ChemRxiv, it is still compliant not to have the data in open access, and this is the case of 15 publications as of January 31, 2024.

Self-assessment of policies of data storage & backup during research

As stated in the MARVEL research data management strategy, day to day work data are either stored on local group resources under the responsibility of the researchers/PIs or on the MARVEL-supported /store partition at CSCS. In fall 2023, each MARVEL group was asked to make a self-assessment of its policies of data storage and backup during research (backup frequency and duration of backup retention) through an online form to be filled by the PI or someone in the group. One third of the groups use the CSCS /store filesystem partition, half the groups use an institutional backup solution, and half the groups use a group-internal backup solution, knowing that more than one solution can be used. The outcomes were good, respecting in principle the minimal requirements of the RDM strategy, namely at least weekly backups and minimum one month backup retention (three months recommended), although some groups need to be reminded of the minimal requirements.

5.5.3 Open access publications

In year 10, we have 128 publications, 98 are published and 30 are available as preprint (mostly on arXiv.org). MARVEL researchers know the SNSF policy concerning the openness of publications and almost all publications (97%) are available on open access. Almost two thirds use the gold road (58 out of 100), the rest use the green road (37 out of 100), depositing the author accepted manuscript either on an institutional repository (currently InfoScience at EPFL, DORA at PSI or Empa, Research Collection at ETH Zurich), or a disciplinary repository (mainly arXiv.org), with apparently no journal requesting an embargo. For the three publications for which the author accepted manuscript is not available in open access yet, the reason is an embargo of 12 months, which is not compliant for two of them — and the groups have been informed of it and that this should be taken into account for the future. The third one is a book chapter, for which a 12-month embargo is allowed.

5.5.4 Open source codes

Developing codes is part of the work of MARVEL researchers, and a key aspect of MARVEL's knowledge transfer is their dissemination as open-source codes. As reported in section 5.2 on Knowledge & Technology Transfer, several new open source codes were released during year 10. Generally, open source codes developed by MARVEL researchers are listed on the MARVEL website.

6 Structural aspects

Tenure-track position in computational materials science at EPFL

The call for the promised tenure-track faculty position in computational materials science has been launched in August 2020 by the EPFL. The selected candidate was announced in October 2021. Prof. Anirudh Raju Natarajan was appointed and started at EPFL in February 2022 as tenure-track assistant professor. He is very committed to MARVEL and already participated actively in phase III.

Tenure-track position between UniFR and PSI

As mentioned in the proposal for phase III, UniFR and PSI were planning to jointly hire in 2022 an assistant professor in the fields of strong light-matter interactions and the computational characterization of light-driven materials, with activities also in the new Laboratory for Materials Simulations at PSI. Prof. Michael Schüler was appointed and started in September 2022. As planned, he is receiving funding from MARVEL within the Advanced Simulation Methods project.

Tenure-track position between maths and materials at EPFL

A proposal for a joint tenure-track professorship between the Institute of Mathematics and the Institute of Materials was conceived by Assyr Abdulle and Nicola Marzari. This received favorable traction and was one of the 3 inter-faculty positions approved by EPFL's direction in 2021 — a search committee identified in 2022 Michael Herbst as the optimal candidate, and he has joined MARVEL and an EPFL professor in May 2023.

Data services

Data storage and services for the Materials Cloud are in place to support the platform till 2036 (i.e., guaranteeing at least 10 years after submission), mostly deployed at CSCS but with a data server also at EPFL and mirroring of the *Archive* on Amazon's AWS.
Federation with the Italian supercomputing center CINECA has taken place as part of the third phase of the EU Centre of Excellence MaX (2022–2026).

Hardware for Materials Cloud

EPFL has committed CHF 150'000 in cash to support hardware for Materials Cloud sustainability to be deployed at EPFL and PSI.

7 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 Publications

All publications have been entered in NIRA, and are listed below with links to the articles (journal and open access links) and, 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 2023 – January 2024.

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

⬢○ D. Santos-Cottin, I. Mohelský, J. Wyzula, F. Le Mardelé, I. Kapon, S. Nasrallah, N. Barišić, I. Živković, J. R. Soh, F. Guo, K. Rigaux, M. Puppin, J. H. Dil, B. Gudac, Z. Rukelj, M. Novak, A. B. Kuzmenko, C. C. Homes, T. Dietl, M. Orlita, and A. Akrap

$EuCd_2As_2$: A Magnetic Semiconductor

Physical Review Letters **131**, 186704 (2023).

Group(s): Akrap / Project(s): DD6

Links to article: Journal / Open access

Related datasets: not applicable

⬢○ F. Le Mardelé, J. Wyzula, I. Mohelsky, S. Nasrallah, M. Loh, S. Ben David, O. Toledano, D. Tolj, M. Novak, G. Eguchi, S. Paschen, N. Barišić, J. Chen, A. Kimura, M. Orlita, Z. Rukelj, A. Akrap, and D. Santos-Cottin

Evidence for three-dimensional Dirac conical bands in TlBiSSe by optical and magneto-optical spectroscopy

Physical Review B **107**, L241101 (2023).

Group(s): Akrap / Project(s): DD6

Links to article: Journal / Open access

Related datasets: not applicable

○ I. Mohelsky, J. Wyzula, B. A. Piot, G. D. Gu, Q. Li, A. Akrap, and M. Orlita

Temperature dependence of the energy band gap in $ZrTe_5$: Implications for the topological phase

Physical Review B **107**, L041202 (2023).

Group(s): Akrap / Project(s): DD6

Links to article: Journal / Open access

Related datasets: not applicable

Group of Giuseppe Carleo

○ D. T. Hoang, F. Metz, A. Thomasen, T. D. Anh-Tai, T. Busch, and T. Fogarty

Variational quantum algorithm for ergotropy estimation in quantum many-body batteries

Physical Review Research **6**, 013038 (2024).

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

Links to article: Journal / Open access

Related datasets: doi.org/10.5281/zenodo.10376853

○ N. Astrakhantsev, G. Mazzola, I. Tavernelli, and G. Carleo

Phenomenological theory of variational quantum ground-state preparation

Physical Review Research **5**, 033225 (2023).

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

Links to article: Journal / Open access

Related datasets: not applicable

G. Gentinetta, D. Sutter, C. Zoufal, B. Fuller, and S. Woerner
Quantum Kernel Alignment with Stochastic Gradient Descent
in *2023 IEEE International Conference on Quantum Computing and Engineering (QCE)* (2023), pp. 256–262.
Group(s): Carleo / Project(s): QS
Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.7804477

Group of Michele Ceriotti

F. Bigi, G. Fraux, N. J. Browning, and M. Ceriotti
Fast evaluation of spherical harmonics with sphericart
The Journal of Chemical Physics **159**, 064802 (2023).
Group(s): Ceriotti / Project(s): P2
Links to article: Journal / Open access
Related datasets: github.com/lab-cosmo/sphericart

N. Lopanitsyna, G. Fraux, M. A. Springer, S. De, and M. Ceriotti
Modeling high-entropy transition metal alloys with alchemical compression
Physical Review Materials **7**, 045802 (2023).
Group(s): Ceriotti / Project(s): P2
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:73-yn

R. K. Cersonsky, M. Pakhnova, E. A. Engel, and M. Ceriotti
A data-driven interpretation of the stability of organic molecular crystals
Chemical Science **14**, 1272 (2023).
Group(s): Ceriotti / Project(s): P2, DD1
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:71-21

A. C. P. Jain, M. Ceriotti, and W. A. Curtin
Natural aging and vacancy trapping in Al-6xxx
Journal of Materials Research **38**, 5171 (2023).
Group(s): Ceriotti, Curtin / Project(s): P1, P2
Links to article: Journal / Open access
Related datasets: not applicable

Group of Clémence Corminboeuf

K. R. Briling, Y. Calvino Alonso, A. Fabrizio, and C. Corminboeuf
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Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:6w-qh

F. Giorgianni, B. Wehinger, S. Allenspach, N. Colonna, C. Vicario, P. Puphal, E. Pomjakushina, B. Normand, and C. Rüegg
Ultrafast frustration breaking and magnetophononic driving of singlet excitations in a quantum magnet
Physical Review B **107**, 184440 (2023).
Group(s): Kenzelmann, Pizzi, Rüegg / Project(s): P4, OSP

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

J. Qiao, G. Pizzi, and N. Marzari
Projectability disentanglement for accurate and automated electronic-structure Hamiltonians
npj Computational Materials **9**, 208 (2023).
Group(s): Marzari, Pizzi / Project(s): P3, P4

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:x0-yf

J. Qiao, G. Pizzi, and N. Marzari
Automated mixing of maximally localized Wannier functions into target manifolds
npj Computational Materials **9**, 206 (2023).
Group(s): Marzari, Pizzi / Project(s): P3, P4

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:2f-hs

Group of Sereina Riniker

M. Thurlemann and S. Riniker
Energy-based clustering: Fast and robust clustering of data with known likelihood functions
The Journal of Chemical Physics **159**, 024105 (2023).
Group(s): Riniker / Project(s): DD1

Links to article: Journal / Open access
Related datasets: github.com/rinikerlab/EnergyBasedClustering

M. Thuerlemann, L. Boselt, and S. Riniker
Regularized by Physics: Graph Neural Network Parametrized Potentials for the Description of Intermolecular Interactions
Journal of Chemical Theory and Computation **19**, 562 (2023).
Group(s): Riniker / Project(s): DD1

Links to article: Journal / Open access
Related datasets: doi.org/10.3929/ethz-b-000549359

Group of Christian Rüegg

F. Giorgianni, B. Wehinger, S. Allenspach, N. Colonna, C. Vicario, P. Puphal, E. Pomjakushina, B. Normand, and C. Rüegg
Ultrafast frustration breaking and magnetophononic driving of singlet excitations in a quantum magnet
Physical Review B **107**, 184440 (2023).
Group(s): Kenzelmann, Pizzi, Rüegg / Project(s): P4, OSP

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

Group of Berend Smit

K. M. Jablonka, P. Schwaller, A. Ortega-Guerrero, and B. Smit
Leveraging Large Language Models for Predictive Chemistry
ChemRxiv. Preprint., to be published in Nature Machine Intelligence (2024), doi:10.26434/chemrxiv-2023-fw8n4-v3.
Group(s): Smit / Project(s): P1

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

H. Gustafsson, M. Kozdra, B. Smit, S. Barthel, and A. Mace
Predicting Ion Diffusion from the Shape of Potential Energy Landscapes
Journal of Chemical Theory and Computation **20**, 18 (2023).
Group(s): Smit / Project(s): P1
Links to article: Journal / Open access
Related datasets: not applicable

P. Gäumann, T. Rohrbach, L. Artiglia, D. Ongari, B. Smit, J. A. van Bokhoven, and M. Ranocchiari
Tandem Hydroformylation-Aldol Condensation Reaction Enabled by Zn-MOF-74
Chemistry–A European Journal **29**, e202300939 (2023).
Group(s): Smit / Project(s): P1
Links to article: Journal / Open access
Related datasets: not applicable

K. M. Jablonka, Q. Ai, A. Al-Feghali, S. Badhwar, J. D. Bocarsly, A. M. Bran, S. Bringuier, L. C. Brinson, K. Choudhary, D. Circi, S. Cox, W. A. de Jong, M. L. Evans, N. Gastellu, J. Genzling, M. V. Gil, A. K. Gupta, Z. Hong, A. Imran, S. Kruschwitz, A. Labarre, J. Lála, T. Liu, S. Ma, S. Majumdar, G. W. Merz, N. Moitessier, E. Moubarak, B. Mouriño, B. Pelkie, M. Pieler, M. C. Ramos, B. Ranković, S. G. Rodriques, J. N. Sanders, P. Schwaller, M. Schwarting, J. Shi, B. Smit, B. E. Smith, J. Van Herck, C. Völker, L. Ward, S. Warren, B. Weiser, S. Zhang, X. Zhang, G. A. Zia, A. Scourtas, K. J. Schmidt, I. Foster, A. D. White, and B. Blaiszik
14 examples of how LLMs can transform materials science and chemistry: a reflection on a large language model hackathon
Digital Discovery **2**, 1233 (2023).
Group(s): Smit / Project(s): P1
Links to article: Journal / Open access
Related datasets: not applicable (review article)

B. Mourino, K. M. Jablonka, A. Ortega-Guerrero, and B. Smit
In Search of Covalent Organic Framework Photocatalysts: A DFT-Based Screening Approach
Advanced Functional Materials **33**, 2301594 (2023).
Group(s): Smit / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.7590815

Group of Ivano Tavernelli

N. Astrakhantsev, G. Mazzola, I. Tavernelli, and G. Carleo
Phenomenological theory of variational quantum ground-state preparation
Physical Review Research **5**, 033225 (2023).
Group(s): Carleo, Tavernelli / Project(s): QS
Links to article: Journal / Open access
Related datasets: not applicable

L. Nagano, A. Miessen, T. Onodera, I. Tavernelli, F. Tacchino, and K. Terashi
Quantum data learning for quantum simulations in high-energy physics
Physical Review Research **5**, 043250 (2023).
Group(s): Tavernelli / Project(s): QS
Links to article: Journal / Open access
Related datasets: not applicable (no data)

A. Nykänen, A. Miller, W. Talarico, S. Knecht, A. Kovyrshin, M. Skogh, L. Tornberg, A. Broo, S. Mensa, B. C. B. Symons, E. Sahin, J. Crain, I. Tavernelli, and F. Pavošević
Toward Accurate Post-Born–Oppenheimer Molecular Simulations on Quantum Computers: An Adaptive Variational Eigensolver with Nuclear-Electronic Frozen Natural Orbitals
Journal of Chemical Theory and Computation **19**, 9269 (2023).
Group(s): Tavernelli / Project(s): QS
Links to article: Journal / Open access
Related datasets: not applicable (no data)

A. Kovyrshin, M. Skogh, A. Broo, S. Mensa, E. Satin, J. Crain, and I. Tavernelli
A quantum computing implementation of nuclear-electronic orbital (NEO) theory: Toward an exact pre-Born–Oppenheimer formulation of molecular quantum systems
The Journal of Chemical Physics **158**, 214119 (2023).
Group(s): Tavernelli / Project(s): QS
Links to article: Journal / Open access
Related datasets: not applicable (no data)

F. Pavošević, I. Tavernelli, and A. Rubio
Spin-Flip Unitary Coupled Cluster Method: Toward Accurate Description of Strong Electron Correlation on Quantum Computers
The Journal of Physical Chemistry Letters **14**, 7876 (2023).
Group(s): Tavernelli / Project(s): QS
Links to article: Journal / Open access
Related datasets: not applicable (no data)

M. John, J. Schuhmacher, P. Barkoutsos, I. Tavernelli, and F. Tacchino
Optimizing Quantum Classification Algorithms on Classical Benchmark Datasets
Entropy **25**, 860 (2023).
Group(s): Tavernelli / Project(s): QS
Links to article: Journal / Open access
Related datasets: not applicable (no data)

M. Rossmannek, F. Pavošević, A. Rubio, and I. Tavernelli
Quantum Embedding Method for the Simulation of Strongly Correlated Systems on Quantum Computers
The Journal of Physical Chemistry Letters **14**, 3491 (2023).
Group(s): Tavernelli / Project(s): QS
Links to article: Journal / Open access
Related datasets: not applicable (no data)

D. J. Egger, C. Capecci, B. Pokharel, P. K. Barkoutsos, L. E. Fischer, L. Guidoni, and I. Tavernelli
Pulse variational quantum eigensolver on cross-resonance-based hardware
Physical Review Research **5**, 033159 (2023).
Group(s): Tavernelli / Project(s): QS
Links to article: Journal / Open access
Related datasets: not applicable (no data)

A. Kovyrshin, M. Skogh, L. Tornberg, A. Broo, S. Mensa, E. Sahin, B. C. B. Symons, J. Crain, and I. Tavernelli
Nonadiabatic Nuclear–Electron Dynamics: A Quantum Computing Approach
The Journal of Physical Chemistry Letters **14**, 7065 (2023).
Group(s): Tavernelli / Project(s): QS
Links to article: Journal / Open access
Related datasets: not applicable (no data)

Group of Vladyslav Turlo

J. F. Troncoso, Y. Hu, N. M. della Ventura, A. Sharma, X. Maeder, and V. Turlo
Machine learning of twin/matrix interfaces from local stress field
Computational Materials Science **228**, 112322 (2023).
Group(s): Turlo / Project(s): P1
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:aj-wq

S. Gramatte, L. P. H. Jeurgens, O. Politano, J. A. Simon Greminger, F. Baras, A. Xomalis, and V. Turlo
Atomistic Simulations of the Crystalline-to-Amorphous Transformation of γ–Al_2O_3 Nanoparticles: Delicate Interplay between Lattice Distortions, Stresses, and Space Charges
Langmuir **39**, 6301 (2023).
Group(s): Turlo / Project(s): P1
Links to article: Journal / Open access (embargo 25.04.2024)
Related datasets: not applicable (review article)

Group of Philipp Werner

V. Christiansson, F. Petocchi, and P. Werner
Correlated electronic structure of $La_3Ni_2O_7$ under pressure
Physical Review Letters **131**, 206501 (2023).
Group(s): Werner / Project(s): ASM
Links to article: Journal / Open access
Related datasets: not applicable

F. Petocchi, J. Chen, J. Li, M. Eckstein, and P. Werner
Photoinduced charge dynamics in $1T-TaS_2$
Physical Review B **107**, 165102 (2023).
Group(s): Werner / Project(s): ASM
Links to article: Journal / Open access
Related datasets: not applicable

Group of Lenka Zdeborová

L. Clarté, B. Loureiro, F. Krzakala, and L. Zdeborová
Expectation consistency for calibration of neural networks
in *Proceedings of the Thirty-Ninth Conference on Uncertainty in Artificial Intelligence*, R. J. Evans and I. Shpitser, eds. (PMLR, 2023), vol. 216 of *Proceedings of Machine Learning Research*, pp. 443–453.
Group(s): Zdeborova / Project(s): P2
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:ws-p3

L. Clarté, B. Loureiro, F. Krzakala, and L. Zdeborová
On double-descent in uncertainty quantification in overparametrized models
in *Proceedings of The 26th International Conference on Artificial Intelligence and Statistics*, F. Ruiz, J. Dy, and J.-W. van de Meent, eds. (PMLR, 2023), vol. 206 of *Proceedings of Machine Learning Research*, pp. 7089–7125.
Group(s): Zdeborova / Project(s): P2
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:zb-71

Phase II PIs, not active in phase III

Group of Ulrich Aschauer

C. Ricca, E. Skoropata, M. D. Rossell, R. Erni, U. Staub, and U. Aschauer
Combined Theoretical and Experimental Study of the Moire Dislocation Network at the $SrTiO_3$-(La,Sr)(Al,Ta)O_3 Interface
ACS Applied Materials & Interfaces **15**, 53678 (2023).
Group(s): Aschauer, Staub / Project(s): DD5
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:ae-cq

C. Ricca, T. Blandenier, V. Werner, X. Wang, S. Pokrant, and U. Aschauer
Conversion of $La_2Ti_2O_7$ to $LaTiO_2N$ via ammonolysis: a first-principles investigation
Physical Chemistry Chemical Physics **25**, 20575 (2023).
Group(s): Aschauer / Project(s): DD5
Links to article: Journal / Open access
Related datasets: not applicable

Group of Claude Ederer

S. Beck and C. Ederer
Interfacial doping in $LaVO_3/SrVO_3$ multilayers from DFT plus DMFT
Physical Review Materials **7**, 055003 (2023).
Group(s): Ederer / Project(s): DD5
Links to article: Journal / Open access
Related datasets: not applicable

Group of Roman Fasel

E. Turco, A. Bernhardt, N. Krane, L. Valenta, R. Fasel, M. Juríček, and P. Ruffieux
Observation of the Magnetic Ground State of the Two Smallest Triangular Nanographenes
JACS Au **3**, 1358 (2023).
Group(s): Fasel / Project(s): DD3
Links to article: Journal / Open access
Related datasets: not applicable

Group of Michel Kenzelmann

D. W. Tam, N. Colonna, N. Kumar, C. Piamonteze, F. Alarab, V. N. Strocov, A. Cervellino, T. Fennell, D. J. Gawryluk, E. Pomjakushina, Y. Soh, and M. Kenzelmann
Charge fluctuations in the intermediate-valence ground state of $SmCoIn_5$
Communications Physics **6**, 223 (2023).
Group(s): Kenzelmann, Pizzi / Project(s): P4, OSP
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:gh-7e

F. Giorgianni, B. Wehinger, S. Allenspach, N. Colonna, C. Vicario, P. Puphal, E. Pomjakushina, B. Normand, and C. Rüegg
Ultrafast frustration breaking and magnetophononic driving of singlet excitations in a quantum magnet
Physical Review B **107**, 184440 (2023).
Group(s): Kenzelmann, Pizzi, Rüegg / Project(s): P4, OSP
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:tm-4t

Group of Titus Neupert

M. O. Soldini, F. Kuester, G. Wagner, S. Das, A. Aldarawsheh, R. Thomale, S. Lounis, S. S. P. Parkin, P. Sessi, and T. Neupert
Two-dimensional Shiba lattices as a possible platform for crystalline topological superconductivity
Nature Physics **19**, 1848 (2023).
Group(s): Neupert / Project(s): DD6
Links to article: Journal / Open access
Related datasets: doi.org/10.6084/m9.figshare.22794413

Group of Marco Ranocchiari

P. Gäumann, D. Ferri, D. Sheptyakov, J. A. van Bokhoven, P. Rzepka, and M. Ranocchiari
In Situ Neutron Diffraction of Zn-MOF-74 Reveals Nanoconfinement-Induced Effects on Adsorbed Propene
The Journal of Physical Chemistry C **127**, 16636 (2023).
Group(s): Ranocchiari / Project(s): DD4
Links to article: Journal / Open access
Related datasets: not applicable

Group of Urs Staub

C. Ricca, E. Skoropata, M. D. Rossell, R. Erni, U. Staub, and U. Aschauer
Combined Theoretical and Experimental Study of the Moire Dislocation Network at the $SrTiO_3$-(La,Sr)(Al,Ta)O_3 Interface
ACS Applied Materials & Interfaces **15**, 53678 (2023).
Group(s): Aschauer, Staub / Project(s): DD5

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

M. Ramakrishnan, Y. Joly, Q. N. Meier, M. Fechner, M. Porer, S. Parchenko, Y. W. Windsor, E. M. Bothschafter, F. Lichtenberg, and U. Staub
Antiferromagnetic spin canting and magnetoelectric multipoles in $h-YMnO_3$
Physical Review Research **5**, 013203 (2023).
Group(s): Staub / Project(s): DD5

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

Group of Anatole von Lilienfeld

B. Huang, O. A. von Lilienfeld, J. T. Krogel, and A. Benali
Toward DMC Accuracy Across Chemical Space with Scalable Δ-QML
Journal of Chemical Theory and Computation **19**, 1711 (2023).
Group(s): VonLilienfeld / Project(s): INC2

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:9p-8a

Group of Oleg Yazyev

D. Gosalbez-Martinez, A. Crepaldi, and O. V. Yazyev
Diversity of radial spin textures in chiral materials
Physical Review B **108**, L201114 (2023).
Group(s): Yazyev / Project(s): DD6

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

S. Zhang, B. Xie, Q. Wu, J. Liu, and O. V. Yazyev
Chiral Decomposition of Twisted Graphene Multilayers with Arbitrary Stacking
Nano Letters **23**, 2921 (2023).
Group(s): Yazyev / Project(s): DD6

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

C. Guo, A. Alexandradinata, C. Putzke, A. Estry, T. Tu, N. Kumar, F.-R. Fan, S. Zhang, Q. Wu, O. V. Yazyev, K. R. Shirer, M. D. Bachmann, H. Peng, E. D. Bauer, F. Ronning, Y. Sun, C. Shekhar, C. Felser, and P. J. W. Moll
Reply to: Low-frequency quantum oscillations in $LaRhIn_5$: Dirac point or nodal line?
Nature Communications **14**, 2061 (2023).
Group(s): Yazyev / Project(s): DD6

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.7724832.

Phase I PIs, not active in phases II and III

Group of Wanda Andreoni

C. Ma, F. Pietrucci, and W. Andreoni
CO_2 Capture and Release in Amine Solutions: To What Extent Can Molecular Simulations Help Understand the Trends?
Molecules **28**, 6447 (2023).
Group(s): Andreoni / Project(s): VP2

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

S. Barison, F. Vicentini, and G. Carleo
Embedding Classical Variational Methods in Quantum Circuits
arXiv:2309.08666 (2023).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: github.com/StefanoBarison/hybrid_ansatz

D. Linteau, S. Barison, N. Lindner, and G. Carleo
Adaptive projected variational quantum dynamics
arXiv:2307.03229 (2023).
Group(s): Carleo / Project(s): QS

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

G. Pescia, J. Nys, J. Kim, A. Lovato, and G. Carleo
Message-Passing Neural Quantum States for the Homogeneous Electron Gas
arXiv:2305.07240 (2023).
Group(s): Carleo / Project(s): P2

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

G. Gentinetta, F. Metz, and G. Carleo
Overhead-constrained circuit knitting for variational quantum dynamics
arXiv:2309.07857 (2023).
Group(s): Carleo / Project(s): QS

Links to article: Journal / Open access
Related datasets: github.com/gentinettagian/circuit-cutting-pvqd

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
arXiv:2302.04919 (2023).
Group(s): Carleo / Project(s): QS

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

Group of Michele Ceriotti

A. Mazitov, M. A. Springer, N. Lopanitsyna, G. Fraux, S. De, and M. Ceriotti
Surface segregation in high-entropy alloys from alchemical machine learning
arXiv:2310.07604 (2023).
Group(s): Ceriotti / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:ps-20

S. N. Pozdnyakov and M. Ceriotti
Smooth, exact rotational symmetrization for deep learning on point clouds
arXiv:2305.19302 (2023).
Group(s): Ceriotti / Project(s): P2

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

L. Gigli, D. Tisi, F. Grasselli, and M. Ceriotti
Mechanism of charge transport in lithium thiophosphate
arXiv:2310.15679 (2023).
Group(s): Ceriotti / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:g2-fp

E. Cignoni, D. Suman, J. Nigam, L. Cupellini, B. Mennucci, and M. Ceriotti
Electronic excited states from physically-constrained machine learning
arXiv:2311.00844 (2023).
Group(s): Ceriotti / Project(s): P2

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

J. Nigam, S. N. Pozdnyakov, K. K. Huguenin-Dumittan, and M. Ceriotti
Completeness of Atomic Structure Representations
arXiv:2302.14770 (2023).
Group(s): Ceriotti / Project(s): P2

Links to article: Journal / Open access
Related datasets: doi.org/10.5281/zenodo.8003293

L. Gigli, A. Goscinski, M. Ceriotti, and G. A. Tribello
Modeling the ferroelectric phase transition in barium titanate with DFT accuracy and converged sampling
arXiv:2310.12579 (2023).
Group(s): Ceriotti / Project(s): P2

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

Group of Clémence Corminboeuf

P. van Gerwen, K. R. Briling, Y. Calvino Alonso, M. Franke, and C. Corminboeuf
Benchmarking machine-readable vectors of chemical re- actions on computed activation barriers
ChemRxiv. Preprint. (2023), doi:10.26434/chemrxiv-2023-0hgbc.
Group(s): Corminboeuf / Project(s): P2

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

Group of Mathieu Luisier

M. Luisier, C. Klinkert, S. Fiore, J. Backman, Y. Lee, C. Stieger, and S. Àron
Field-Effect Transistors Based on 2D Materials: A Modeling Perspective
in *Beyond-CMOS: State of the Art and Trends*, A. Cresti, ed. (Wiley-ISTE, 2023), pp. 33–78.
Group(s): Luisier / Project(s): ASM

Links to article: Book / Open access (submitted version)
Related datasets: not applicable (review article)

Group of Nicola Marzari

T. Chiarotti, A. Ferretti, and N. Marzari
Energies and spectra of solids from the algorithmic inversion of localized GW
arXiv:2302.12193 (2023).
Group(s): Marzari / Project(s): P4
Links to article: Journal / Open access
Related datasets: not applicable

D. Grassano, N. Marzari, and D. Campi
High-throughput screening of Weyl semimetals
arXiv:2308.01663 (2023).
Group(s): Marzari / Project(s): P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:9t-f8

L. Bastonero and N. Marzari
Automated all-functionals infrared and Raman spectra
arXiv:2308.04308 (2023).
Group(s): Marzari / Project(s): P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:90-36

E. Gazzarrini, R. K. Cersonsky, M. Bercx, C. S. Adorf, and N. Marzari
The rule of four: anomalous stoichiometries of inorganic compounds
arXiv:2307.14742 (2023).
Group(s): Marzari / Project(s): P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:fm-za

M. Vanzini and N. Marzari
Towards a minimal description of dynamical correlation in metals
arXiv:2309.12144 (2023).
Group(s): Marzari / Project(s): P4
Links to article: Journal / Open access
Related datasets: not applicable

N. Rivano, N. Marzari, and T. Sohier
Density-functional perturbation theory for one-dimensional systems: implementation and relevance for phonons and electron-phonon interactions
arXiv:2310.03907 (2023).
Group(s): Marzari / Project(s): DD3
Links to article: Journal / Open access
Related datasets: not applicable

L. Ponet, E. Di Lucente, and N. Marzari
The Energy Landscape of Magnetic Materials
PREPRINT available at Research Square (2023), doi:10.21203/rs.3.rs-3358581/v1.
Group(s): Marzari / Project(s): P4
Links to article: Journal / Open access
Related datasets: not applicable

S. Gelin, N. E. Kirchner-Hall, R. R. Katzbaer, M. J. Theibault, Y. Xiong, W. Zhao, M. M. Khan, E. Andrewlavage, P. Orbe, S. M. Baksa, M. Cococcioni, I. Timrov, Q. Campbell, H. Abruña, R. E. Schaak, and I. Dabo
Ternary oxides of s- and p-block metals for photocatalytic solar-to-hydrogen conversion
arXiv:2303.03332 (2023).
Group(s): Marzari / Project(s): P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:zh-14

C. Cignarella, D. Campi, and N. Marzari
Searching for the thinnest metallic wire
arXiv:2312.16968 (2023).
Group(s): Marzari / Project(s): P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:9a-p9

E. Macke, I. Timrov, N. Marzari, and L. C. Ciacchi
Orbital-resolved DFT+ U for molecules and solids
arXiv:2312.13580 (2023).
Group(s): Marzari / Project(s): P4
Links to article: Journal / Open access
Related datasets: not applicable

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
ChemRxiv. Preprint. (2023), doi:10.26434/chemrxiv-2023-4vs5w.
Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: doi.org/10.24435/materialscloud:qh-gt

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
The Wannier-Functions Software Ecosystem for Materials Simulations
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Group(s): Marzari, Pizzi / Project(s): P3, P4
Links to article: Journal / Open access
Related datasets: not applicable

Group of Giovanni Pizzi

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Related datasets: doi.org/10.24435/materialscloud:qh-gt

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The Wannier-Functions Software Ecosystem for Materials Simulations
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Group(s): Marzari, Pizzi / Project(s): P3, P4

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

Group of Michael Schüler

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

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

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Group of Vladyslav Turlo

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

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

Links to article: Journal / Open access
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3. Publications involving several groups or several projects (inter-group or inter-project)

C. Ricca, E. Skoropata, M. D. Rossell, R. Erni, U. Staub, and U. Aschauer
Combined Theoretical and Experimental Study of the Moire Dislocation Network at the $SrTiO_3$-(La,Sr)(Al,Ta)O_3 Interface
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Phenomenological theory of variational quantum ground-state preparation
Physical Review Research **5**, 033225 (2023).
Group(s): Carleo, Tavernelli / Project(s): QS
Links to article: Journal / Open access
Related datasets: not applicable

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Natural aging and vacancy trapping in Al-6xxx
Journal of Materials Research **38**, 5171 (2023).
Group(s): Ceriotti, Curtin / Project(s): P1, P2
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Related datasets: not applicable

D. W. Tam, N. Colonna, N. Kumar, C. Piamonteze, F. Alarab, V. N. Strocov, A. Cervellino, T. Fennell, D. J. Gawryluk, E. Pomjakushina, Y. Soh, and M. Kenzelmann
Charge fluctuations in the intermediate-valence ground state of $SmCoIn_5$
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F. Giorgianni, B. Wehinger, S. Allenspach, N. Colonna, C. Vicario, P. Puphal, E. Pomjakushina, B. Normand, and C. Rüegg
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Links to article: Journal / Open access
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C. Hsu, M. Rohde, G. Borin Barin, G. Gandus, D. Passerone, M. Luisier, P. Ruffieux, R. Fasel, H. S. J. van der Zant, and M. El Abbassi
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Related datasets: not applicable

W. Huang, O. Braun, D. I. Indolese, G. Borin Barin, G. Gandus, M. Stiefel, A. Olziersky, K. Müllen, M. Luisier, D. Passerone, P. Ruffieux, C. Schönenberger, K. Watanabe, T. Taniguchi, R. Fasel, J. Zhang, M. Calame, and M. L. Perrin
Edge Contacts to Atomically Precise Graphene Nanoribbons
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Links to article: Journal / Open access
Related datasets: not applicable

N. Krane, E. Turco, A. Bernhardt, D. Jacob, G. Gandus, D. Passerone, M. Luisier, M. Juríček, R. Fasel, J. Fernández-Rossier, and P. Ruffieux
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Nano Letters **23**, 9353 (2023).
Group(s): Luisier, Passerone / Project(s): ASM
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npj Computational Materials **9**, 208 (2023).
Group(s): Marzari, Pizzi / Project(s): P3, P4
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Related datasets: doi.org/10.24435/materialscloud:x0-yf

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D. Campi, N. Mounet, M. Gibertini, G. Pizzi, and N. Marzari
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ACS Nano **17**, 11268 (2023).
Group(s): Marzari, Pizzi / Project(s): P3, P4

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Related datasets: doi.org/10.24435/materialscloud:36-nd

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How to verify the precision of density-functional-theory implementations via reproducible and universal workflows
Nature Reviews Physics **6**, 45 (2024).
Group(s): Marzari, Pizzi / Project(s): P3, P4

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Cover picture

Wannier-BSE (right) vs experiments (left). Top: Polarization-averaged time-resolved ARPES signature of excitons in monolayer WSe_2. Bottom: Circular dichroism with respect to the pump pulse polarization. The positive-negative pattern of the dichroism directly reflects the Berry curvature in each valley (groups of Michael Schüler, PSI and UniFR and Philipp Werner, UniFR).
Reference: 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*, arXiv:2308.09634 (2023).

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