MARVEL

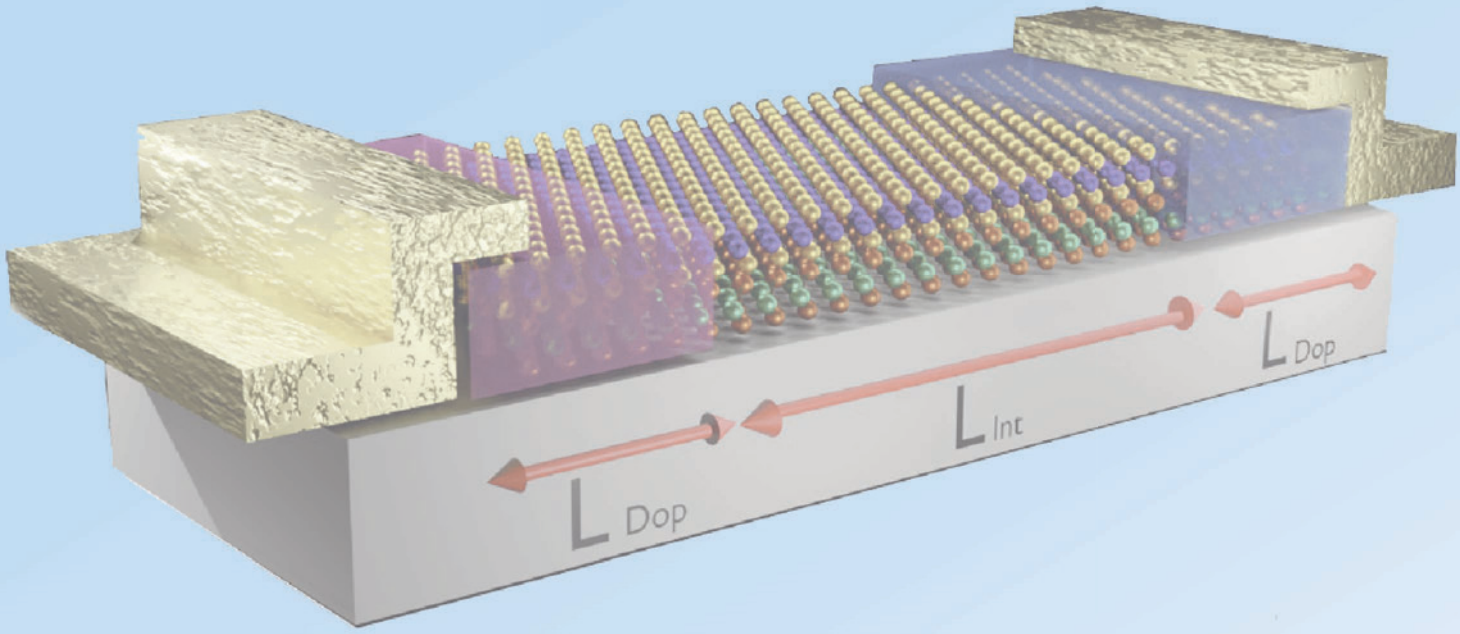
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Materials' Revolution: Computational Design and Discovery of Novel Materials

Progress Report

Year 9

February 2022 - January 2023



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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 MARVEL NCCR has now started its last 4-year phase, and has, at the same time, very successfully established a phase-in of structural efforts that will continue beyond the end of the project. These take place most notably thanks to the embedding of its activities at PSI, Empa, and CSCS, that, as national centers integrating research and services, provide the timescale and long-term planning that are needed. In fact, the entire vision for the project relies also on the concept of digital infrastructures as a counterpart for computational science of established models for major experimental facilities: from particle accelerators, synchrotrons and free-electron lasers to telescopes, antennas' arrays, and satellites. While the role, relevance and impact of computational science is prominently present in all scientific and technological indicators, the development model for it is mostly absent or is just emerging, and with MARVEL we want to contribute, propel and establish this vision and need for computational science — to the broader research community, policymakers, and funders.

On the research front, EPFL has made key assistant-professor hires in Materials, Math and Materials, and Quantum Technologies, and PSI and UniFR in Materials Simulations: Light-Matter Interactions, ensuring a lively long-term research environment for the field.

We highlight below some of the key research and structural developments — at our recent and very successful retreat in Grindelwald the message was passed to all PIs that *usability* and *visibility* of the algorithms, codes, and tools underpinning research will be key metrics for 2022–2026.

Pillar 1 The overarching theme of Pillar 1 is the identification of new attractive materials for targeted applications from among millions of possible compounds/compositions. In the area of novel metals, a first demonstration of the path to achieving this goal has been accomplished for the BCC HEAs. Refinements to the path are now in progress. The thrust in metals also continues to push forward the use of machine learned interatomic potentials to answer complex metallurgical questions, especially in lightweight metals. For the metal-organic frameworks, the AiiDA workflows to predict the adsorption properties have been integrated into a platform that seamlessly integrates process design, techno-economics, and life-cycle analysis. This platform allows us to assess the carbon avoidance cost of a carbon capture process that uses a particular MOF, together with a complete life-cycle analysis.

Pillar 2 Building on the methodological and software development work in phase II, the team in Pillar 2 has at the same time advanced the fundamental investigation and analysis of the mathematical and physical foundations of atomistic machine learning, and begun the process of integrating different software components into a coherent, modular infrastructure.

Pillar 3 Pillar 3 develops the infrastructure to enable exascale-ready accessible materials simulations-as-a-service, combining turnkey workflows (in AiiDA) with accelerated codes implementing novel robust algorithms (in SIRIUS). In year 9, it demonstrated the scalability of the infrastructure to drive high-throughput simulations filling one the largest pre-exascale machines (LUMI). 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 Laboratory for Materials Simulations has been created at PSI — it is headed by Prof. Nicola Marzari, and it includes three groups: Materials Software and Data (Dr. Giovanni Pizzi), Multiscale Materials Modelling (Dr. Matthias Krack) and Light-Matter interactions (Prof. Michael Schüler). PSI and Empa are working closely together on the development of AiiDAlab, and of turnkey workflows for the automated calculation of materials properties.

Novel efforts have been ignited also to expand the scope of the MARVEL digital infrastructure, with funded collaborations for the integration of electronic laboratory notebooks and expansion at Empa to applications in atmospheric science.

Advanced Simulation Methods The goal of the Advanced Simulation Methods projects is to develop powerful simulation methods for studying the equilibrium and non-equilibrium properties of moderately and strongly correlated materials and devices. This includes the development at ETH Zurich and Empa of a toolset for simulating transport through nanodevices, the further development of the GW+DMFT *ab initio* approach at UniFR, and the exploration of light-matter coupled systems at PSI and UniFR. Common to all these efforts is the use of diagrammatic techniques based on (non-equilibrium) Green's functions.

Quantum Simulations The Quantum Simulations project is working on hybrid quantum algorithms to combine classical and quantum computing for more accurate electronic structure calculations. The project's initial phase focuses on quantum embedding techniques and integration with classical methods with different costs and accuracy, such as DFT, Neural Quantum States, and Density Matrix Embedding Theory (DMET). Software integration between the software CP2K, Qiskit, and NetKet has successfully started and sets the ground for the next phase.

Structure-related aspects The flagship event for the community was the Psi-k 2022 conference, held at EPFL, with more than 1'300 participants. This was a great success, and greatly contributed to presenting Switzerland and EPFL as a very exciting and innovative environment for the field. All our other structural activities, from the summer schools and camps to the workshops, as well as the online footprint (greatly enhanced by the CECAM partnerships in the Classics, Mary Ann Mansigh conversations, and the Lhumos portal) are going strong, as is the Materials Cloud portal and the NCCR website. The efforts in equal opportunities now cover even more broadly underrepresented groups — from the INSPIRE Potentials fellowships and the #NCCRWomen campaign to the ASESMAnet and ExAf initiatives for African researchers, both also supported generously attendance of 20 researchers to Psi-k 2022.

2 Reaction to the recommendations of the review panel

The reactions to the full proposal were very enthusiastic:

The review panel considers that the NCCR MARVEL has been a huge success and that the team should be congratulated for their remarkable achievements in terms of scientific advances but also on the collaborative nature of the project at large. The proposal for phase III is clear, coherent, with excellent attention to details. The future plans clearly build on the elements of the NCCR which are expected to have the most long-term impact, and therefore the panel commends the way projects have been selected and prioritized. The proposal is further considered to be incredibly strong, exciting and possessing a very high potential to achieve a truly impactful theoretical/computational user facility. The panel sees no reason to doubt that excellent science as well as software tools will continue to be produced in phase III, and therefore supports the full proposal without reservation.

One question was asked on the bonus project:

Regarding the bonus project, the panel acknowledges that wanting to include a hardware angle makes perfect sense, and therefore opting for a project in quantum technology is an obvious choice. However, its integration in MARVEL's activities is not clear yet, and neither is the way the PIs are going to collaborate. The panel also regrets that the description of the bonus project did not contain references to other similar efforts already made by other research groups in the world.

with the recommendation

The panel supports the bonus project, which has excellent scientific potential and is very topical. However, the bonus project should focus more on aspects that are relevant for MARVEL in order to be better integrated in the NCCR's activities to ensure tight collaborations between research groups.

There is already a very close integration between the activities of IBM and UZH, and the broad plan on algorithms and software for materials discovery has been further discussed at the Grindelwald retreat and will be presented at the site visit in March. With the arrival of key new PIs at EPFL and in Switzerland in quantum technologies (both on the theoretical, algorithmic, and experimental sides) we believe even more that this was the best area in which to ignite new efforts. Also, at the policymaking level, Switzerland is investing in major efforts on hardware and on software and algorithms (at PSI, at ETH Zurich, at UniGE, and last but not least with EPFL's Center for Quantum Science and Engineering, jointly funding Carleo and Marzari with a start-up grant).

3 NCCR Organisation

3.1 Structure and organisation of the NCCR, management activities

3.1.1 Structure of the NCCR

In phase III, MARVEL's mission revolves around the following six core activities, spread over the following six projects, as also represented in Fig. 1:

Pillar 1 – Design and Discovery of Novel Materials, dedicated to the projects that have shown a combination of scientific and economic impact — metal-organic frameworks and alloys for additive manufacturing.

Pillar 2 – Machine Learning Platform for Molecules and Materials, dedicated to developing and exploiting the capabilities of machine learning for molecules and materials through universal machine-learning models, data-augmented quantum calculations, active-learning workflows, and automatic data exploration.

Pillar 3 – Digital Infrastructure of Open Simulations and Data, dedicated to continuing building the open-source digital infrastructure that will power the MARVEL legacy, including the Materials Cloud, AiiDA/AiiDAlab, and the transition of HPC codes on future architectures.

Pillar 4 – Long-term Integration in the Swiss Scientific Landscape, dedicated to ensuring the long-term establishment of the MARVEL mission in the Swiss ecosystem and the continuation of the post-2026 ac-

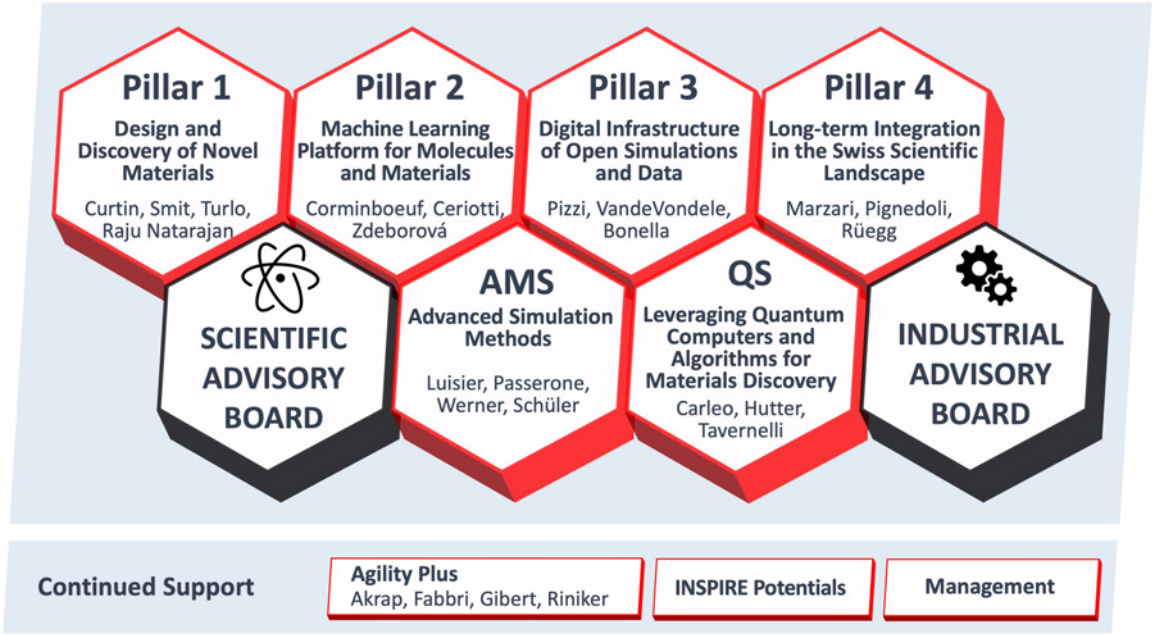

Figure 1: *Organization of MARVEL in phase III.*

tivities, in close collaboration with the national laboratories (PSI, Empa), that become intellectual and sustainable hubs for state-of-the-art materials simulations.

Advanced Simulation Methods project dedicated to the integration of the methodological efforts on correlated materials and on devices that have started already in phase II.

Quantum Simulations project – Leveraging Quantum Computers and Algorithms for Materials Discovery, the Bonus project in the proposal for phase III, dedicated to the algorithms and the interfacing and leveraging of classical digital computers with quantum computers for the two goals of materials simulations and materials data mining.

Along with the director, Nicola Marzari (EPFL and PSI), Clémence Corminboeuf and Michele Ceriotti (both at EPFL) are the deputy directors, and Sara Bonella (EPFL) and Joost VandeVondele (CSCS) complete the Executive Committee in charge of day-to-day activities and of strategic decisions (reallocation of funding, establishment and termination of projects).
The Scientific Committee is composed of the Executive Committee and all project leaders; it has the formal role of discussing the science and an advisory role on strategy. Meetings take place when convened by the Executive Committee, or at the request of 3 project leaders.
EPFL is the leading house and the other institutions involved in phase III are PSI, Empa, ETH Zurich, CSCS, UniFR, UZH and IBM.
A Scientific Advisory Board (SAB), chaired by Giulia Galli (University of Chicago), and an Industrial Advisory Board (IAB), chaired by Erich Wimmer (Materials Design), provide feedback on all activities.

3.1.2 Organisation of the NCCR

As mentioned in the full proposal for phase III, UniFR and PSI pledged to jointly hire 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. The MARVEL director was also involved, as part of the search committed, and the search led to hiring Michael Schüler, joining both UniFR in September 2022 and PSI in January 2023 as Group Leader for Light-Matter Interactions in the Laboratory for Materials Simulations there. Michael is also part of MARVEL as group leader in the Advanced Simulation Methods project.
EPFL has hired new junior professors — Zoë Holmes and Michael Herbst — that are very fitting to MARVEL topics. Discussions are ongoing on their possible integration into MARVEL, using also some of the Agility Plus funding planned for phase III. In particular, Michael Herbst hire was possible 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. This was enthusiastically endoresed and led to the current hire.
On the management side, the team is established, with Lidia Favre-Quattropani at 60% as scientific manager, Patrick Mayor at 100% as program manager, Carey Sargent at 20% in charge of written communication for the website and the social media, Ursula Vaucher at 80% as financial officer, and Cornelia Bujenita at 80% as administrative assistant. This year, the MARVEL management, and especially the program manager, drove and coordinated the Psi-k 2022 conference, which was a great showcase for EPFL and Switzerland (with more than 1'300 attendees — see section 5.2 on Knowledge & Technology Transfer for the details).
The MARVEL data team was adapted to the projects of phase III perserving the objective to broadly represent the different projects and institutions.

3.1.3 Activities and measures

Events organisation

In year 9, since February 2022, MARVEL management organized meetings, lectures and events, described in chapter 5. We mention, for example:

- MARVEL stand and presentation at Thematic day for high school students, gymnasium in Thun, April 7.
- MARVEL phase II closing event, April 28.
- MARVEL phase II kick-off event, April 29.
- Mary Ann Mansigh conversation, Erich Wimmer (Materials Design), EPFL, May 5.
- Meeting of MARVEL with a Swissnex delegation at PSI, May 17.
- Summer camp for high school students *Des atomes aux ordinateurs, à la découverte de la programmation scientifique*, EPFL, June 27–July 1.
- Swiss Equivariant Learning Workshop, EPFL, July 11–14
- Psi-k 2022 conference, Lausanne, August 22–25.
- MARVEL booth at Psi-k 2022 conference, Lausanne, August 22–25.

- MARVEL conference fellowships for Psi-k 2022 conference.
- MARVEL stand at PSI's Open Doors Day, PSI, October 23.
- AiiDA plug-in developers hackathon 2022, EPFL, Novembre 21–22.
- Online Executive Committee Meeting, November 8.
- EPFL Information days for high-school students, visit of labs, EPFL, November 25.
- MARVEL Review and Retreat, January 18–20, 2023, Grindelwald.
- Executive committee meeting, January 19, Grindelwald.
- INSPIRE Potentials — MARVEL Master's Fellowships for female Master's students, with 2 calls in April and October.
- 1 week of #NCCRWomen portraits on social networks, November 14–18.
- Organization of several #NCCRWomen in-school visits, planned from January 2023.
- 4 online or hybrid MARVEL distinguished lectures, Sharon Glotzer (Univ. Michigan), February 8, Garnet Chan (Caltec), April 5, Alán Aspuru-Guzik (Univ. Toronto), May 31, and Heather Kulik (MIT), December 13.
- 2 online CECAM-MARVEL Classics in molecular and materials modeling lectures, Giorgio Parisi (Universitá di Roma la Sapienza) and Marc Mézard (Universitá Bocconi Milano), November 3, and Antoine Georges (Flatiron Institute & Collège de France) and Gabriel Kotliar (Rutgers University & Brookhaven National Lab.), December 8.
- 2 online junior seminars in February and March 2022.
- 2 seminars at EPFL.
- 16 online one-to-one meetings between the MARVEL director and the phase III PIs, several slots in October.

Other events

In addition, in year 9, MARVEL members organized at least 17 conferences, tutorials or workshops, either in person or online; MARVEL sponsored 3 of these.

Measures

The MARVEL Research Data Management strategy was updated for phase III, sent to the SNSF for validation end of May, and then shared with all MARVEL members.
The NCCR has also been asked to prepare a document presenting our communication plans in case a crisis were to arise. This document, including various scenarios, has been finalized at the end of 2022, and has been shared with the various communication departments of institutions involved in MARVEL.

MARVEL is currently discussing and preparing an updated version of its internal regulations, that will be valid for phase III.

3.2 Status of collaboration / integration and added-value

3.2.1 Status of collaborations and integration

At the NCCR level

The teams working in the different pillars have achieved, in part thanks to the work in the previous years, an excellent level of synergy and organization, and many of the long-term structural collaborations wouldn't have happened at all without MARVEL — these, e.g., include the efforts of Pillar 1 (Curtin/Raju Natarajan/Turlo), Pillar 2 (Corminboeuf/Ceriotti), Pillar 3 (Pizzi/VandeVondele), Pillar 4 (PSI and Empa), ASM (Luisier/Passerone, and Passerone/Werner). These are complemented by a very fitting bonus 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: Bonella, interacting with SIRIUS/VandeVondele in Pillar 3; Schüler, with Werner in ASM. Last, as mentioned, discussions with Holmes (Quantum Simulations) and Herbst (Pillar 3) have started or will start as soon as they join.

At the national level

The key platform players of phase I (PSI, Empa, CSCS) have not only been close partners across MARVEL, but allow to transition the effort in the post-2026 landscape — with the creation of the Scientific Computing, Theory and Data division at PSI, where the Laboratory for Materials Simulations is, the structural consolidation of the Empa computational activities (for which an effort has started — similar to that of PSI — in terms of long-term organization and planning), and the established partnership with CSCS in delivering a platform-as-a-service through the Materials Cloud.

At the international level

The core partners have been MaX, the EU Centre of Excellence for e-infrastructure on Ma-

terials 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 a planned federation of the *Archive* from 2023 onwards), 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 being built to push automatically data on the Materials Cloud when they become open access. Also, it 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.

3.2.2 Added value

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

3.3 Changes to the consortium's composition

As listed in the full proposal, 7 new PIs joined at the beginning of phase III: Raju Natarajan, Turlo, Zdeborová, Bonella, Pignedoli, Schüler, and Carleo. Computational PIs of phase II that are no longer present in phase III (also due to the fact that phase III funding is 60% of the previous period) are Goedecker, Parrinello (moved to Genova, Italy), Pasquarello, Spaldin, Ederer, Aschauer (soon at PLUS University, Salzburg, Austria), Yazyev, Soluyanov (tragically passed away), Neupert, Laino, von Lilienfeld (moved to Toronto, Canada), and Roth.

4 Research

4.1 Highlights from year 8

Advances in machine learning, modeling and experiment all play an important role in our drive to accelerate the design and discovery of novel materials. In year 8, we made significant progress in each of these aspects. Selected papers below were chosen among those on which we wrote our science highlights for the MARVEL website.

4.1.1 Advances in machine learning

Machine learning models of matter beyond interatomic potentials

Combining electronic structure calculations and machine learning (ML) techniques has become commonplace in atomistic modeling. ML interatomic potentials, e.g., can now describe the potential energy surface of a material across many phases, including a wide range of defects. Looking ahead, ML models that can predict properties beyond the interactions between atoms might eventually allow integrated machine learning models to replace costly electronic structure calculations entirely. In a *Nature* paper [1] researchers including EPFL's Michele Ceriotti took a step in that direction with a new ML framework for predicting the electronic density of states (DOS).

Learning the exciton properties of azo-dyes

Machine learning techniques have demonstrated their accuracy at retrieving excited-state properties of large molecular datasets at a reduced computational cost, however, the models tend to be specialized in targeting individual properties. As an alternative, researchers in the Corminboeuf group have designed a framework for machine learning transition densities and the corresponding hole and particle densities of molecules, based on a SA-GPR model for the ground-state electron density [2]. Using a dataset of 3'427 azo-heteroarene photoswitches, they show the advantages of this approach and use the predictions of these fundamental properties to obtain chemically relevant features, including the state character and the exciton topological descriptors such as the extent of the push-pull signature.

Machine learning cracks oxidation states of crystal structures

EPFL chemical engineers including Berend Smit developed a ML model that can predict a compound's oxidation state, which is generally predicted by bond valence theory. This doesn't always work, however, especially in materials with crystal structures. In a *Nature Chemistry* paper [3] the researchers showed how they were able to train a machine learning algorithm to categorize metal-organic frameworks by oxidation state.

Manifolds in commonly used atomic fingerprints lead to failure in machine learning four-body interactions

The existence of manifolds in two atomic environment fingerprints commonly used to characterize the local environments of atoms in ML and other contexts causes a failure to machine learn four-body interactions such as torsional energies, which are an important part of standard force fields. No such manifolds can be found for the Overlap Matrix (OM) fingerprint due to its intrinsic many-body character, making it an appealing alternative, researchers

from the Goedecker group at UniBas found in a *Journal of Chemical Physics* paper [4].

Comprehensive electronic-structure methods review

Nicola Marzari, Andrea Ferretti and Chris Wolvertion published a in-depth review on "Electronic-structure methods for materials design" as an "Insight" piece in *Nature Materials* [5]. They provides an overview of electronic-structure and machine-learning methods (Fig. 1), discusses their application to the prediction of materials properties, and examines different strategies used to target the broader goals of materials design and discovery. Looking ahead, the authors consider emerging challenges in the predictive accuracy of the calculations, and in addressing the real-life complexity of materials and devices. They also stress the importance of the computational infrastructures that support such research, and how the planning for funding these and the supporting career models is only just beginning to emerge.

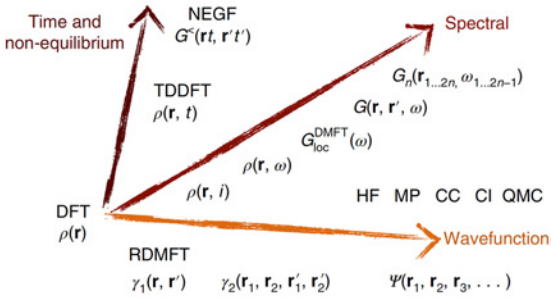

Figure 1: *The complex landscape of electronic-structure methods.*

4.1.2 Advances in modeling

Solving the inverse materials design problem with alchemical chirality

Combing through the vast set of all possible stable combinations of elements and structural configurations is a daunting task in materials design. A paper in *Science Advances* from von Rudorff and von Lilienfeld at UniBas [6] showed how the concept of 4-dimensional chirality resulting from an alchemical reflection plane in the nuclear charge space allows researchers to break down combinatorial scaling. This alchemical chirality and its simplifications deepen our understanding of chemical compound space and enable researchers to establish new trends on the fly, without resorting to empirical observation.

Landau levels serve as probe for band topology in graphene Moiré superlattices

Researchers led by EPFL's Oleg Yazyev determined a straightforward way of probing the topological character of electronic bands in two-dimensional Moiré superlattices using Landau level sequences. The results, published in *Physical Review Letters* [7], can be easily extended to other twisted graphene multilayers and h-BN/graphene heterostructures, making the approach a powerful tool for detecting nontrivial valley band topology (Fig. 2).

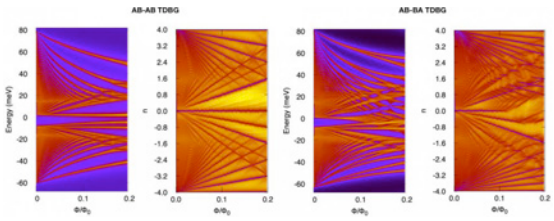

Figure 2: *Landau levels and Wannier diagrams for the flatband manifold in the AB-AB (left) and AB-BA (right) configurations of twisted double bilayer graphene at twist angle θ of 1.89 degrees.*

Common workflows for computing material properties with various quantum engines

Using electronic-structure simulations based on density-functional theory to predict material properties has become routine, thanks at least in part to an ever-widening choice of increasingly robust simulation packages. The wide range of methods, algorithms and paradigms available makes it difficult, however, for non-experts to select or efficiently use any one for a given task. In a *npj Computational Materials* paper involving MARVEL teams of Smit, Marzari and Pizzi [8], researchers showed how developing common interfaces for workflows that automatically compute material properties address these challenges, demonstrating the approach with an implementation involving 11 different simulation codes.

Ab initio model of Ca_2RuO_4 perovskite in remarkably good agreement with available experimental data

Researchers in Werner's group at UniFR tested the GW + EDMFT *ab initio* approach for correlated materials modeling. Using the insulator-metal transition in the perovskite Ca_2RuO_4 as a benchmark, they found that their parameter-free simulation was in close agreement with

the available experimental data and that the extension to the nonlocal polarization and self-energy provided by GW are essential to attaining such accuracy. The calculations published in *Physical Review B* [9] represent an important test and an encouraging result for the further application and development of the GW + EDMFT framework.

Superconductivity, high critical temperature found in 2D semimetal W_2N_3

Two-dimensional superconductors have drawn considerable attention both for the fundamental physics they display as well as for potential applications in fields such as quantum computing. Although considerable efforts have been made to identify them, materials with high transition temperatures have been hard to find. Materials that feature both superconductivity and non-trivial band topology, a combination that could potentially give rise to exotic states of matter, have proven even more elusive. In their paper in *Nano Letters* [10], researchers in Marzari's group have now predicted just such a material in the easily exfoliable, topologically non-trivial 2D semimetal W_2N_3.

Polarons free from many-body self-interaction in density functional theory

Polarons can affect numerous phenomena in a material but have been difficult to model correctly. In their *Physical Review Letters* paper [11], EPFL researchers Stefano Falletta and Alfredo Pasquarello advance the conceptual understanding of the self-interaction problem in density functional theory, paving the way to efficient calculations of polarons in large systems, in systematic studies involving large sets of materials, and in molecular dynamics evolving over long time periods (Fig. 3).

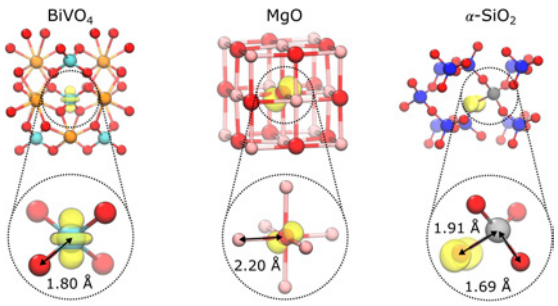

Figure 3: *Polaron isodensity surface*

4.1.3 Advances in experiment

Low-temperature crystallization of phase-pure alpha-formamidinium lead iodide

Perovskite solar cells are among the most promising and cheapest photovoltaic technologies now available, but widespread application has been hampered by issues linked to long-term stability and processability. Now, researchers including Michele Parrinello have addressed this problem in their *Science Advances* paper [12] with a combined experimental and simulation study that could improve the design of industrial-scale processing techniques for $MAPbI_3$ and $FAPbI_3$, two lead perovskites.

ARPES gives first observation of dispersive excitons in a low-dimensional metallic system

Already used in some solar cells, excitons, with their charge neutrality and expected mobility, have also been proposed as potential transmitters of quantum information. In either use, it's essential to understand how and why these quasiparticles move. Investigations into exciton mobility have been inaccessible to traditional optical experiments though because they only create and detect excitons with negligible momentum. Now, using angle-resolved photoemission spectroscopy (ARPES), scientists, including MARVEL groups of Shi and Yazyev, have detected several types of mobile excitons in the quasi-one-dimensional metallic trichalcogenide, $TaSe_3$, reported in their *Nature Materials* paper [13]. They've also shown that certain exciton properties can be tuned by surface doping.

On-surface synthesis and characterization of nitrogen-substituted undecacenes

Heteroatom substitution can be used to tailor the electronic, magnetic, and physico-chemical properties of acenes. With potential applications in organic electronics, this fine-tuning could allow for precise engineering and property optimization. Synthesizing and characterizing larger acenes has, however, remained a challenge for solution chemistry because they feature low solubility and high reactivity. Researchers at Empa addressed this by demonstrating first on-surface synthesis of three undecacene analogs substituted with four nitrogen atoms on an Au(111) substrate and then characterizing the materials using various techniques. The work published in *Nature Communication* [14] paves the way towards

the precise fabrication of nitrogen-substituted acenes and their analogs, potential building-blocks of organic electronics and spintronics.

First-ever rare earth nickelate single crystals lead to first experimental evidence supporting predicted multiferroicity

Perovskites have drawn much attention for potential applications in fields of research ranging from optoelectronics, to battery engineering and neuromorphic computation, but crucial experimental data needed to validate theoretical predictions has been lacking. The materials are very difficult to synthesize and, to date, it has not been possible to grow sizable bulk single crystals based on rare earths other than La, Pr and Nd. Now, PSI researchers from the Medarde group and colleagues have successfully grown bulk single crystals of the full nickelate family [15] while another team has used them to provide experimental evidence supporting the existence of multiferroicity in these materials [16] (Fig. 4).

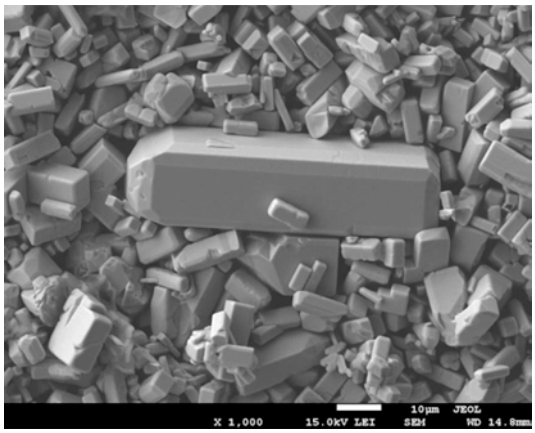

Figure 4: *$RNiO_3$ nickelate crystals grown in lab*

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. L. Deringer, N. Bernstein, G. Csányi, C. Ben Mahmoud, M. Ceriotti, M. Wilson, D. A. Drabold, and S. R. Elliott, *Origins of structural and electronic transitions in disordered silicon*, Nature **589**, 59 (2021).
- [2] 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).
- [3] K. M. Jablonka, D. Ongari, S. M. Moosavi, and B. Smit, *Using collective knowledge to assign oxidation states of metal cations in metal-organic frameworks*, Nature Chemistry **13**, 771 (2021).
- [4] B. Parsaeifard and S. Goedecker, *Manifolds of quasi-constant SOAP and ACSF fingerprints and the resulting failure to machine learn four-body interactions*, The Journal of Chemical Physics **156**, 034302 (2022).
- [5] N. Marzari, A. Ferretti, and C. Wolverton, *Electronic-structure methods for materials design*, Nature Materials **20**, 736 (2021).
- [6] G. F. von Rudorff and O. A. von Lilienfeld, *Simplifying inverse materials design problems for fixed lattices with alchemical chirality*, Science Advances **7**, eabf1173 (2021).
- [7] Q. Wu, J. Liu, Y. Guan, and O. V. Yazyev, *Landau Levels as a Probe for Band Topology in Graphene Moiré Superlattices*, Physical Review Letters **126**, 056401 (2021).
- [8] S. P. Huber, E. Bosoni, M. Bercx, J. Bröder, A. Degomme, V. Dikan, K. Eimre, E. Flage-Larsen, A. Garcia, L. Genovese, D. Gresch, C. Johnston, G. Petretto, S. Poncé, G.-M. Rignanese, C. J. Sewell, B. Smit, V. Tseplyaev, M. Uhrin, D. Wortmann, A. V. Yakutovich, A. Zadoks, P. Zarabadi-Poor, B. Zhu, N. Marzari, and G. Pizzi, *Common workflows for computing material properties using different quantum engines*, npj Computational Materials **7**, 136 (2021).
- [9] F. Petocchi, V. Christiansson, and P. Werner, *Fully ab initio electronic structure of Ca_2RuO_4*, Physical Review B **104**, 195146 (2021).
- [10] D. Campi, S. Kumari, and N. Marzari, *Prediction of Phonon-Mediated Superconductivity with High Critical Temperature in the Two-Dimensional Topological Semimetal W_2N_3*, Nano Letters **21**, 3435 (2021).
- [11] S. Falletta and A. Pasquarello, *Many-Body Self-Interaction and Polarons*, Physical Review Letters **129**, 126401 (2022).
- [12] P. Ahlawat, A. Hinderhofer, E. A. Alharbi, H. Lu, A. Ummadisingu, H. Niu, M. Invernizzi, S. M. Zakeeruddin, M. I. Dar, F. Schreiber, A. Hagfeldt, M. Grätzel, U. Rothlisberger, and M. Parrinello, *A combined molecular dynamics and experimental study of two-step process enabling low-temperature formation of phase-pure alpha-FAPbI(3)*, Science Advances **7**, eabe3326 (2021).
- [13] J. Ma, S. Nie, X. Gui, M. Naamneh, J. Jandke, C. Xi, J. Zhang, T. Shang, Y. Xiong, I. Kapon, N. Kumar, Y. Soh, D. Gosálbez-Martínez, O. V. Yazyev, W. Fan, H. Hübener, U. D. Giovannini, N. C. Plumb, M. Radovic, M. A. Sentef, W. Xie, Z. Wang, C. Mudry, M. Müller, and M. Shi, *Multiple mobile excitons manifested as sidebands in quasi-one-dimensional metallic $TaSe_3$*, Nature Materials **21**, 423 (2022).
- [14] K. Eimre, J. I. Urgel, H. Hayashi, M. Di Giovannantonio, P. Ruffieux, S. Sato, S. Otomo, Y. S. Chan, N. Aratani, D. Passerone, O. Gröning, H. Yamada, R. Fasel, and C. A. Pignedoli, *On-surface synthesis and characterization of nitrogen-substituted undecacenes*, Nature Communications **13**, 511 (2022).
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- [16] I. Ardizzone, J. Teyssier, I. Crassee, A. B. Kuzmenko, D. G. Mazzone, D. J. Gawryluk, M. Medarde, and D. van der Marel, *Raman spectroscopic evidence for multiferroicity in rare earth nickelate single crystals*, Physical Review Research **3**, 033007 (2021).

4.2 Results from year 9

Pillar 1 Design and Discovery of Novel Materials

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

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

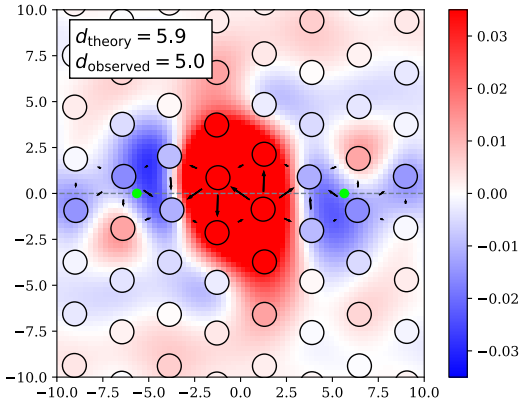
1 Progress of the different efforts

1.1 Design of novel metals

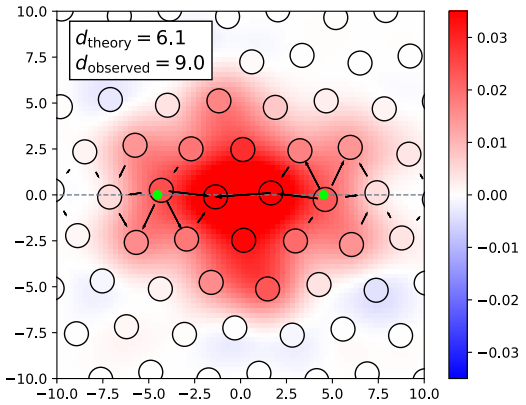
In the area of design of novel metal alloys, there are major accomplishments to report in the areas of (i) design of high entropy alloys (HEAs), (ii) development of neural network interatomic potentials (NNPs), and (iii) applications of NNPs that advance quantitative understanding of metals.

We have executed a computationally-driven alloy design strategy to discover new refractory high-temperature BCC high entropy alloys that have (i) high strength at high temperature, (ii) high melting point, (iii) a wide temperature range of single-phase stability, (iv) low density, and (v) prospects for useful ductility [1]. The overall approach uses our recent theory for strength vs temperature, the Calphad method for predicting phase behavior and melting points, and a surrogate model for capturing ductility trends. The search identified the Hf-Mo-Nb-Ta-Ti family as the only suitable quinaries, with 10 candidate alloys. Leinenbach has fabricated and tested one designed alloy, achieving broadly good agreement with predictions. Eliminating high-density Ta, we identified $\sim$ 10 alloys in the Hf-Mo-Nb-Ti family with even better properties.

The Hf-Mo-Nb-Ti family is now the focus of further study to predict and understand thermodynamics and performance at a more-detailed level, and thus establish a general path for computationally-guided alloy design of BCC HEAs. We have created a large DFT database of alloy energies for binary, ternary, and quarternary alloys of Hf-Mo-Nb-Ti in the BCC, B2, and various Laves phases. Curtin and Raju Natarajan are using this database to train both a traditional cluster expansion (CE) and a new NNP, and the convex hulls of both CE and NNP are being investigated. Future work will use these methods in Monte Carlo studies of phase behavior and short-range-order, and the database will be extended to include data for modeling plasticity and fracture in attractive alloys. Raju Natarajan has launched a study of the thermodynamics of the Al-Nb-Ta-Ti-V-Zr, with new insights into the forma-



(a) Prismatic I-w Plane



(b) Pyramidal I-w Plane

Figure 1: *Nye tensor and differential displacement maps showing the prismatic and pyramidal* $\langle \mathbf{a} \rangle$ *screw dislocations in pure Zr. Consistent with experiments, (i) the prismatic screw is stable relative to the pyramidal screw and the NNP predicts a very small energy difference of 3.8 meV/A in excellent agreement with the DFT value of 3.2 meV/A, and (ii) the basal screw is unstable (not shown).*

tion of a high-temperature disordered B2 Al-Ti-Zr precipitate phase observed experimentally. Significant progress has also been made on verifying new theory, and unexpected features, of the effects of short-range-order on alloy strength. Finally, we have further validated our strength theories using targeted binary alloys (FCC AuNi, with Yin (Zhejiang); BCC Mo-Ti, with Heilmeier and Kauffmann (KIT); papers submitted).

In collaboration with Materials Design, we have completed work on an NNP for hcp Zr [2]. This NNP captures subtle but essential features of Zr, especially (i) the relative stability of $\langle \mathbf{a} \rangle$ screw dislocations on competing glide planes (Fig. 1) and (ii) accurate fracture behaviors for many different crack/crystal orientations, which is usually the most challenging issue for machine learned potentials. The NNP has been extended to Zr-H with very good results for key hydride phases and their fracture behavior, which is essential for simulations of Zr failure in H environments. Curtin and Turlo are developing an NNP for the Cu-W system to enable modeling of nanoscale Cu-W multilayer materials studied at Empa, with follow-up work on Cu-Mo. Turlo and Curtin will develop a machine learning potential for the Ti-B system, identified as the most promising system for aiding unique Empa capabilities in directed-energy-deposition of metal/nanoparticle materials. They will start with a Ti database and machine learned potential newly developed by Raju Natarajan.

The MARVEL NNPs for Mg have been used to gain new insight into unusual prismatic slip in pure hcp Mg at low temperatures ($T < 200$ K) [3]. The prismatic yield stress is independent of temperature, which defies expectations of thermally-activated plastic flow. We have shown that each individual NNP has an instability for prismatic glide at some critical stress, where the prismatic screw, normally unstable to a transformation to a lower-energy basal-dissociated structure, glides on the prism plane. One particular NNP (NNP-77) has a critical stress of 100 MPa in excellent agreement with both experiments and new large-scale DFT studies (B. Yin, former MARVEL member)(Fig. 2). The previously unexplained behavior is now understood atomistically, and agrees with experiments (Fig. 3). Theoretically, the instability is consistent with the (not rigorous) principle of maximum energy dissipation rate which posits that dynamical systems will evolve in the direction of maximum energy dissipation rate, which here is prism glide driven by an applied shear stress. In other work,

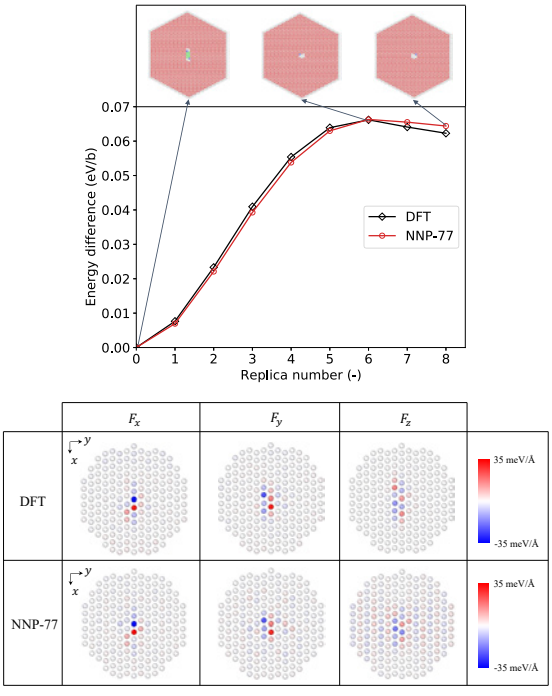


Figure 2: *Comparison of NNP-77 and DFT energies and forces for prismatic slip in Mg. No information on prismatic slip was included in the training set of NNP-77. Top: Energy vs replica for the path between an initial basal-dissociated $\langle \mathbf{a} \rangle$ screw dislocation (replica 0) and the final prism $\langle \mathbf{a} \rangle$ screw, as predicted by very large (2'000 atom) DFT and NNP-77. Bottom: atomic forces on individual atoms at replica 7, as predicted by DFT and NNP-77. The overall agreement is exceptionally good.*

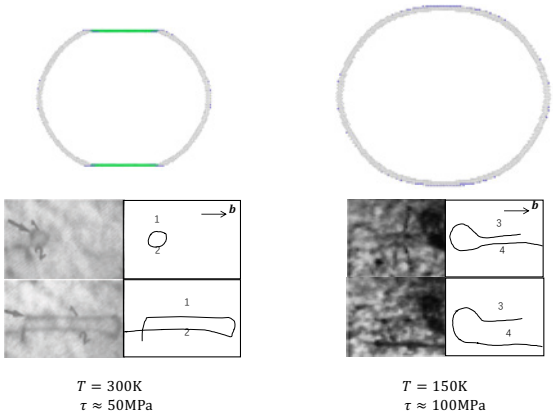


Figure 3: *Prismatic loop expansion at high T/low stress (left) and low T/high stress (right), as observed in MD simulations using the NNP (top) and as observed experimentally (bottom). At high T/low stress, the screw segments dissociate on the basal plane (green) and do not glide while at low T/high stress the loop expands in all directions, with no dissociation onto the basal plane, due to the prism screw slip instability.*

we have used a Mg-Zn binary NNP, emerging from our MARVEL Al-Cu-Mg-Zn NNP for Al alloys, to guide the DFT investigation of Zn solute effects on prism slip in Mg-Zn alloys.

1.2 Discovery of novel metal-organic frameworks

In this part of the project, we focussed on three questions:

1. How to diversify the database of metal-organic frameworks (MOFs)?
2. How to link the Cambridge Structural Database (CSD) that contains the crystal structures with the NIST database that has the isotherms?
3. How to optimize the yield of the MOF synthesis?

By combining metal nodes and organic linkers, an infinite number of metal-organic frameworks (MOFs) can be designed *in silico*. Therefore, when making new databases of such hypothetical MOFs, we need to ensure that they not only contribute toward the growth of the count of structures but also add different chemistries to the existing databases. We designed a database of circa 20'000 hypothetical MOFs, which are diverse in terms of their chemical design space — metal nodes (Fig. 4), organic linkers, functional groups, and pore geometries [4]. Using machine learning techniques, we visualized and quantified the diversity of these structures. We find that by adding the structures of our database, the overall diversity metrics of hypothetical databases improve, especially in terms of the chemistry of metal nodes. We then assessed the usefulness of diverse structures by evaluating their performance, using grand-canonical Monte Carlo simulations, in two important environmental applications — post-combustion carbon capture and hydrogen storage. We find that many of these structures perform better than widely used benchmark materials such as Zeolite-13X (for post-combustion carbon capture) and MOF-5 (for hydrogen storage). All the structures developed in this study, and their properties, are provided on the Materials Cloud *Archive* [5] to encourage further use of these materials for other applications.

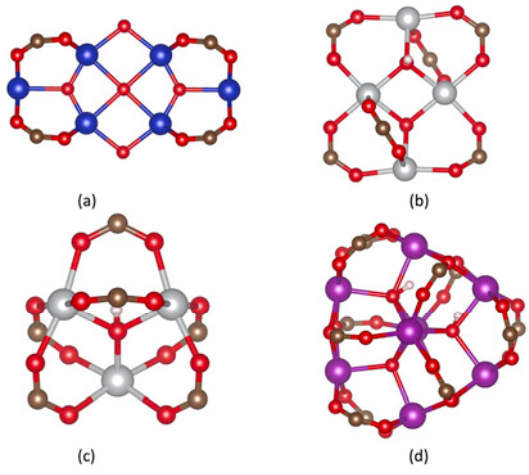


Figure 4: *Some metal nodes used in this study to generate hypothetical MOFs. (a) An 8-connected Co metal node, (b) a 6-connected Zn metal node, (c) a 6-connected Ni metal node, and (d) a 12-connected Mn metal node. These metal nodes are shown to highlight different metals, connectivities, and geometries used in this study.*

Computational screening techniques have long been an important part of the scientific toolbox to study MOFs. However, a broad validation of molecular simulations in these materials is impeded by the lack of a connection between databases of gas adsorption experiments and databases of the atomic crystal structure of corresponding materials. We aim to connect the gas adsorption isotherms of metal-organic frameworks collected in the NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials to the corresponding crystal structures in the Cambridge Structural Database (CSD). With tens of thousands of isotherms and crystal structures reported to date, an automatic approach is needed to establish this link [6]. As a first application and consistency check, we compare the pore volume measured from low-temperature argon or nitrogen isotherms to the geometrical pore volume computed from the crystal structure. Overall, 545 argon or nitrogen isotherms could be matched to a corresponding crystal structure. We find that the pore volume computed via the two complementary methods shows the subset of isotherms measured on these materials as a seed study. One of the interesting outcomes of this study was a graph theory-based approach to identify similar structures in the CSD (Fig. 5).

The synthesis of metal-organic frameworks (MOFs) is often complex, and the desired structure is not always obtained. We developed a joint machine learning and experimental approach to optimize the synthesis conditions of Al-PMOF [7]. Al-PMOF is a promising material for carbon capture applications. It was previously synthesized using a hydrothermal reaction, which gave a low throughput yield due to its relatively long reaction time (16 hours). Here, we use a genetic algorithm to systemat-

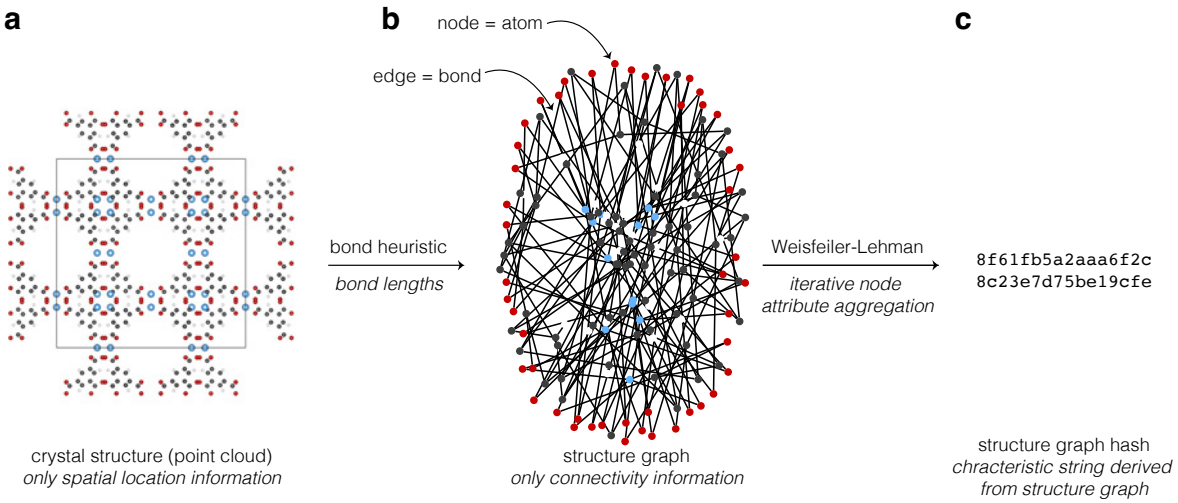


Figure 5: *From crystal structure (a) to structure graph hash (c). The crystal structure specifies the location of atoms in three dimensional space. First, a periodic structure graph (b) is created based on heuristic bond length thresholds. This graph no longer contains information about the positions but only about the connectivity (shown as black edges) between the atoms (shown as blue nodes), thus making it robust against small changes in the atom positions or cell dimensions. Second, we use the Weisfeiler-Lehman algorithm to aggregate information about the neighborhood of each node and compute a characteristic fixed-length hash of the graph. Comparing two graphs for identity then reduces to comparing their structure graph hash.*

ically search for the optimal synthesis conditions and a microwave-based high-throughput robotic platform for the syntheses. We show that, in just two generations, we could obtain excellent crystallinity and yield close to 80% in a much shorter reaction time (50 minutes). Moreover, by analyzing the failed and partially successful experiments, we could identify the most important experimental variables that determine the crystallinity and yield (Fig. 6).

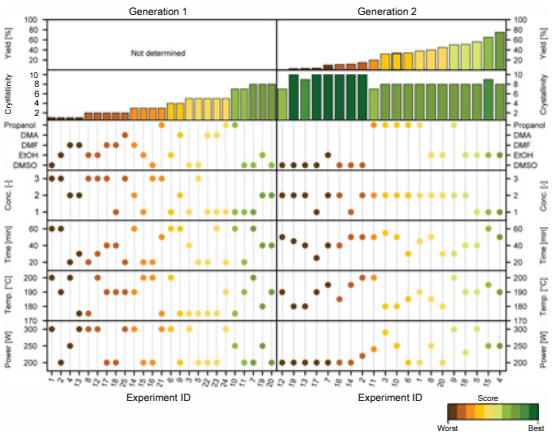


Figure 6: *Parameters and optimization results for each synthesis of generations 1 and 2. Each experimental variable studied (i.e. microwave power, reaction temperature, time, concentration, and solvents) selected for each AI-PMOF synthesis are depicted by circles, while the bar graphs illustrate the ranking of each reaction in terms of crystallinity and yield. The color code is given for the worst (brown) and best (dark green) samples. Generation 1 was ranked in terms of the crystallinity of each sample, while the yield determined the success of generation 2 as all samples proved to be highly crystalline.*

2 Contribution to overall goals and initial proposal

2.1 Design of novel metals

The project continues to advance computational paths for design and discovery that are central to the overall MARVEL goal. At the same time, the methods are being used to advance fundamental metallurgical understanding beyond the existing knowledge in the field. This is being achieved using new approaches (machine learning potentials) and devising innovative mechanistic concepts.

2.2 Discovery of novel metal-organic frameworks

In this period, we have focused on developing various workflows to streamline the materials discovery process. We created an ecosystem for machine learning of MOFs. The idea of this ecosystem is that we provide a reference set of MOFs and reference data such that machine learning studies can be more easily compared. In addition, this ecosystem has a set of tools to prevent data leakage and have all kind of options to evaluate the performance.

3 Collaborative and interdisciplinary components

3.1 Design of novel metals

The AiiDA workflow developed previously continues to be used by new MARVEL team members. We are developing additional automated tools for computing relevant metallurgical issues, mainly defect structures each of which requires special geometries and boundary conditions. Collaborations among the main co-PIs, and with external colleagues, has been noted in the technical discussion. Overall the team is making excellent progress toward achieving the overall goals of the project. Collaborations with Empa experimental efforts are proceeding.

3.2 Discovery of novel metal-organic frameworks

The AiiDA workflow that has been developed to screen materials for carbon capture applications has been integrated into the PrISMa-platform. In the platform, the AiiDA workflow generates the basic data for over 1'000 materials. This data is the input for different process models that describe the carbon capture process. The process data is input for a techno-economic evaluation, and for a life-cycle analysis. The platform then allows us to evaluate the carbon avoidance costs of each of these 1'000 materials depending on the source of the CO_2 (natural gas, coal, or cement), the region in the world (UK, USA, China, or Switzerland), and the CO_2 sink. This highly interdisciplinary work is done in collaboration with Heriot-Watt University, UC Berkeley, ETH Zurich, and the Ecole Normale in Paris.

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] M. Liyanage, D. Reith, V. Eyert, and W. A. Curtin, *Machine learning for metallurgy V: A neural-network potential for zirconium*, Physical Review Materials **6**, 063804 (2022).
- [3] 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).
- [4] S. Majumdar, S. M. Moosavi, K. M. Jablonka, D. Ongari, and B. Smit, *Diversifying Databases of Metal Organic Frameworks for High-Throughput Computational Screening*, ACS Applied Materials & Interfaces **13**, 61004 (2021).
- [5] S. Majumdar, S. M. Moosavi, K. M. Jablonka, D. Ongari, and B. Smit, *Diversifying databases of metal organic frameworks for high-throughput computational screening*, Materials Cloud Archive **2021.126** (2021), doi:10.24435/materialscloud:yn-de.
- [6] D. Ongari, L. Talirz, K. M. Jablonka, D. W. Siderius, and B. Smit, *Data-Driven Matching of Experimental Crystal Structures and Gas Adsorption Isotherms of Metal-Organic Frameworks*, Journal of Chemical & Engineering Data **67**, 1743 (2022).
- [7] N. P. Domingues, S. M. Moosavi, L. Talirz, K. M. Jablonka, C. P. Ireland, F. M. Ebrahim, and B. Smit, *Using genetic algorithms to systematically improve the synthesis conditions of Al-PMOF*, Communications Chemistry **5**, 170 (2022).

List of year 9 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).

⬢○ Y. Hu and W. A. Curtin
Modeling of precipitate strengthening with near-chemical accuracy: case study of Al-6xxx alloys
Acta Materialia **237**, 118144 (2022).
Group(s): Curtin / Project(s): P1
Related datasets: doi.org/10.24435/materialscloud:9m-4n

⬢○ 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).
Group(s): Curtin / Project(s): P1
Related datasets: doi.org/10.24435/materialscloud:3f-w3

⬢○ M. Liyanage, D. Reith, V. Eyert, and W. A. Curtin
Machine learning for metallurgy V: A neural-network potential for zirconium
Physical Review Materials **6**, 063804 (2022).
Group(s): Curtin / Project(s): P1
Related datasets: doi.org/10.24435/materialscloud:vy-02

⬢○ Y. Rao, C. Baruffi, A. D. Luca, C. Leinenbach, and W. A. Curtin
Theory-guided design of high-strength, high-melting point, ductile, low-density, single-phase BCC high entropy alloys
Acta Materialia **237**, 118132 (2022).
Group(s): Curtin / Project(s): P1
Related datasets: doi.org/10.24435/materialscloud:a4-yf

⬢○ N. P. Domingues, S. M. Moosavi, L. Talirz, K. M. Jablonka, C. P. Ireland, F. M. Ebrahim, and B. Smit
Using genetic algorithms to systematically improve the synthesis conditions of Al-PMOF
Communications Chemistry **5**, 170 (2022).
Group(s): Smit / Project(s): P1
Related datasets: doi.org/10.5281/zenodo.7186602

⬢○ D. Ongari, L. Talirz, K. M. Jablonka, D. W. Siderius, and B. Smit
Data-Driven Matching of Experimental Crystal Structures and Gas Adsorption Isotherms of Metal-Organic Frameworks
Journal of Chemical & Engineering Data **67**, 1743 (2022).
Group(s): Smit / Project(s): P1
Related datasets: github.com/danieleongari/matching_isodb_csd

Pillar 2 — Machine Learning Platform for Molecules and Materials

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

Partners: Lenka Zdeberová (EPFL), Giuseppe Carleo (EPFL)

1 Progress of the different efforts

During the first six months of year 9, Pillar 2 launched the effort aiming at deploying a general and robust machine learning platform for molecules and materials. Following the objectives we had set forward for this research thrust, we have both advanced the conceptual understanding of the machine learning (ML) frameworks for materials modeling (with a focus on the aspects with a direct impact on materials design) and on the development of an easy-to-use, modular and efficient software library.

1.1 Sampling and materials design

During the first part of the third phase, the Pillar 2 team continued its efforts to demonstrate the use of ML-powered sampling of configurations to advance materials design and discovery. Following a previous collaboration leveraging neural network potentials to describe chemical reactions in complex environment, the Corminboeuf and Ceriotti groups performed a comparative study of two complementary machine learning architectures and sampling approaches to address the challenging task of learning the potential energy surfaces PES (DFT level) of oligopeptides trained on smaller organic fragments [1], demonstrating converged and transferable sampling of the conformational landscape of complex and flexible tripeptides with comparable accuracy and computational cost.

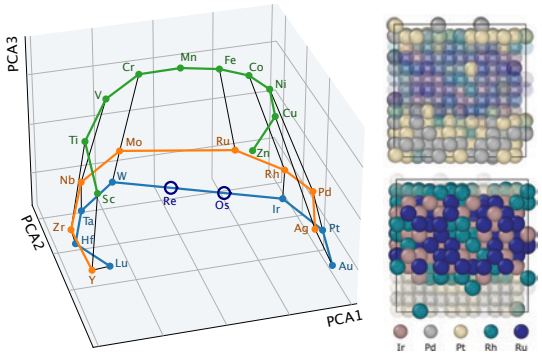


Figure 1: *Left: Top-3 principal components of the alchemical coupling matrix for the 25 transition metals included in our HEA model. The periods are highlighted with red, yellow and blue lines, and the columns are indicated by black thin lines. The model provides also semi-quantitative predictions for elements that are* not *included in the train set, whose weights can be obtained by interpolating the neighboring species in the periodic table (e.g. Re and Os, indicated with empty circles in the figure). Right: A snapshot of a simulation of an equimolar IrPdPtRuRh alloy, which is being studied for applications in catalysis, and that is shown to have a tendency to phase-separate into PdPt and IrRuRh regions.*

The physically-motivated framework that underlies these simulations is also beneficial to achieve an intuitive understanding of the behavior of complex organic systems. In a recent study, the Ceriotti team tailored the atom-centred representations for the task of predicting the binding energy in organic solids and then used the resulting models to attribute different stabilizing effects to different chemical moieties [2]. This study is also notable for leveraging the Materials Cloud infrastructure and the chemiscope software [3] to provide an interface[1] to inspect this dataset, serving as a resource for experimental and computational collaborators to design new molecular solids for a broad range of applications, including for pharmaceutical or optoelectronics.

Another example of how the team is leveraging the methodological advances achieved in phase II to tackle challenging materials-science problems is the development of a universal forcefield for transition-metal high entropy alloys, based on the alchemical compression scheme of [4]. The idea is to avoid the increase in memory and computational footprint of ML potentials with increasing number of species by representing elements as vector in a low-dimensional space of pseudo-elements. As shown in Fig. 1, these vectors, which are obtained in a data-driven manner in the process of training the potential, reflect intuitive similarities across the periodic table. By training the model on a dataset of 25'000 high en-

[1] Available at https://molmotifs.matcloud.xyz

tropy alloys (HEAs)-like structures containing 25 different d-block elements, we could predict the energy and forces of arbitrary alloys with any of the 25 element with test set accuracy of 10 meV/atom for the energies and 200 meV/Å for the forces, which is enough to verify the thermodynamic stability of alloys that are relevant for applications to catalysis. This line of research is being pursued with an industrial grant from BASF, and has also clear relevance for the metallurgical materials design in Pillar 1.

1.2 Machine learning beyond structures and potentials

Most physics-based machine learning models rely upon the use of structural information as inputs, and use them to predict the interatomic potential. We have worked to extend this established paradigm in different directions. On one side, we have developed and applied models that use descriptors based on purely structural information to predict functional properties of materials, that are associated with the electronic state of the system, or with its response to an external perturbation. For example, the Ceriotti group has proposed a symmetry-adapted framework to predict single-particle Hamiltonians and energy levels [5], and used a ML model of the ground-state electron density [6, 7] to build an approximation of the Mermin free-energy functional to describe the behavior of electrons at finite temperature, up to the extreme conditions found in an astrophysical context [8]. In collaboration with the Marzari and Pizzi groups, it was also demonstrated how an integrated model that describes simultaneously the interatomic potential and the polarization makes it possible to compute bulk thermodynamic and dielectric properties of a prototypical ferroelectric, namely barium titanate ($BaTiO_3$) [9].

On another front, we demonstrated the use of descriptors that go beyond a mere representation of the atomic positions, that limits the general property predictions of quantum systems owing to the injectivity problem (two molecules having the same geometry but different charge or spin should not have the same representation). To address this problem, the Corminboeuf group introduced the SPectrum of Approximate Hamiltonian Matrices (SPA^HM) [10], a class of representations incorporating information from light-weight one-electron Hamiltonians, typically used to start the self-consistent field (SCF) quantum chemical computations. These representations that

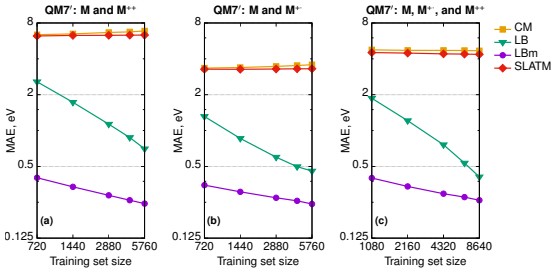


Figure 2: *Learning curves of kernel ridge regression models based on different representations on a QM7 subset including charged and radical cation species. CM and SLATM are geometry-based representations, while LB and LBm are SPA^HM representations with different approximate Hamiltonians.*

intrinsically account for charge and spin multiplicity were shown to perform well on datasets characterized by a wide variation of charge and spin, for which the traditional structure-based representations fail (Fig. 2).

As a third effort, and in collaboration with the Quantum Simulations project, the Carleo team has been working on developing neural network-based representations of many-body interacting fermions. Specifically, continuous-space neural quantum state (NQS) framework has been introduced, that is suitable for the simulation of periodic systems. The ansatz uses a message passing architecture on a graph that inherently implements the indistinguishability of same-species quantum particles. This architecture allows reducing the number of variational parameters by one to two orders of magnitude compared to currently used NQS for continuous space, while reaching comparable or better accuracy. This architecture is being exploited to study the equilibrium properties of the electron gas and will be extended to study materials *ab initio*.

1.3 The M-stack platform for machine learning in molecules and crystals

The groups of Ceriotti and Corminboeuf launched a unified M-stack platform, which integrates software packages from both groups in an interoperable, easily accessible and robust manner. There are currently three distinct blocks connected in M-stack: in-house representations for molecules and materials (SOAP, SPA^HM, etc.), methods for computing suitable loss functions, and machine learning models.

a) *Equistore* The equistore package[2] enables storing atomistic machine learning data, in-

[2]Equistore source code is available online at https://github.com/lab-cosmo/equistore

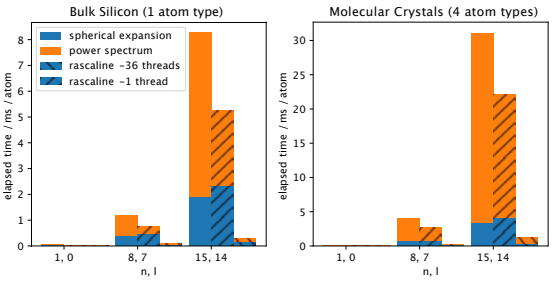


Figure 3: *Timing for the calculation of SOAP power spectrum and its gradients in rascaline (hatched bars), compared to single-threaded librascal (plain bars).*

cluding all the metadata required to correctly interpret the data. It is used as a standard input and output format to connect the different components of M-stack. Individual components are thus inter-exchangeable such as streamlined pipelines can be constructed using any combination.

b) *Rascaline* Rascaline is the module that takes in atomic systems, and computes their machine learning representations as efficiently as possible. It is a successor to our first prototype code librascal [11], made to use CPU parallelism. Improvements in the calculation time can be seen in Fig. 3.
Rascaline also contains an implementation of the LOng Distance Equivariants (LODE) representation [12], incorporating exact long-distance terms (behaving like $1/r$ or $1/r^6$) into a local representation. This allows to use the same code base and infrastructure to build more complex physically inspired machine learning models.

c) *Q-stack* The Q-stack module deals with specific tasks for molecular machine learning. It is especially well suited for predicting scalar fields expressed using gaussian basis functions, routinely used in quantum chemistry. Current capabilities include quick basis set optimization, computation of integrals between gaussian type orbitals required for loss computation (e.g. overlap matrices, Coulomb matrices), calculation of local charges from scalar fields (e.g. Hirshfeld charges), scalar field decompositions and generation of the SPA$^{\mathrm{H}}$M family of representations from molecular coordinates. All the functionalities are fully connected to M-stack through equistore interfaces. The Q-stack module, installation instructions, examples and tests are available online[3].

[3] https://github.com/lcmd-epfl/Q-stack

1.4 Data analytics, automation and active learning

Facilitating the availability, interoperability and storage of datasets has been essential to both the development of cost-efficient machine learning methods and the high-throughput computational screening of molecules and materials. In connection with this effort and with the prospect of constructing database featuring a variety of charge and spin states (see above), the Corminboeuf team introduced the *cell2mol* algorithm [13], which provides a reliable and comprehensive interpretation of all molecular species contained in crystallography files (including the connectivity and charge) in a deterministic manner (Fig. 4). Ultimately, *cell2mol* provides all the necessary information to automatize QC computations or to set up the training of ML models. Its performance was assessed by constructing eight different databases of transition metal complexes with a variety of charges as well as a database of 13k unique ligands with all the necessary information to exploit them in molecular assemblers. Using *cell2mol*, the Cambridge Structural Database, also mined for organocatalyst structures, was leading to the largest and most diverse database of organocatalyst structures to date [14] available on the Materials Cloud [15]. *cell2mol* is now being deployed as a web app in the Materials Cloud server such as to enable the interpretation and labeling of any molecular crystal unit cell with the aim of building molecular datasets. Note that the algorithm [13] is also adapted to the reverse task that consists in combining isolated charged molecules into a charge-neutral molecular crystal.
To facilitate the analysis of large dataset we also released a new version of chemiscope [3], that allows using the visualizer as an iPython widget that can be loaded in a notebook alongside the code that processes atomic structures and data.
Finally, we have devoted efforts to uncertainty

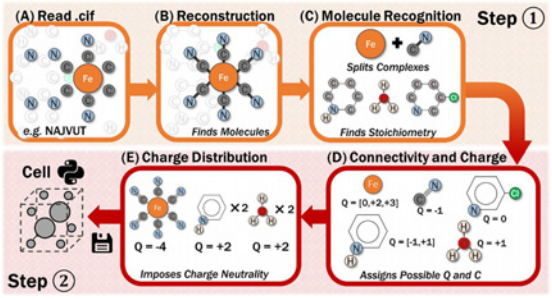


Figure 4: *Simplified workflow of cell2mol.*

quantification, which is a central challenge in reliable and trustworthy machine learning and has been a focus of phase II [16]. The Zdeborová group is performing comparisons between popular uncertainty measures for binary classification in a mathematically tractable high-dimensional model for over-parametrized neural networks, and is currently extending this work to regression so as to provide better-calibrated uncertainty measures.

2 Contribution to overall goals and initial proposal

Several of the core software components that are needed to complete the software integration that is one of the main goals of this Pillar (i-PI, rascaline/librascal, Q-stack, chemiscope, equistore) have been released in their development version, as discussed above. Ease of usability and interoperability has been prioritized throughout. As of now, it constitutes a head-start towards the goal of M-stack, the full-fledged, open-source and sustainable ecosystem which will act as the foundation of future research efforts for researchers inside and outside Pillar 2 and MARVEL.
With the support of matching-funds activities, the team has also advanced the foundational efforts on understanding the structure of leading ML frameworks, and on the incorporation of ML ingredients into quantum chemistry and electronic-structure workflows and vice versa.

3 Collaborative and interdisciplinary components

The groups taking part in the activities of this Pillar have been in constant contact throughout this first part of phase III, and are currently working to prepare a demonstrative workflow that combines Q-stack and equistore to streamline training and inference for models of the electronic charge density. Collaborations with other groups within and outside MARVEL are ongoing, and resulted in several joint publications [9, 17].

MARVEL publications

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

- [1] R. Fabregat, A. Fabrizio, E. A. Engel, B. Meyer, V. Juraskova, M. Ceriotti, and C. Corminboeuf, *Local kernel regression and neural network approaches to the conformational landscapes of oligopeptides*, Journal of Chemical Theory and Computation **18**, 1467 (2022).
- [2] R. K. Cersonsky, M. Pakhnova, E. A. Engel, and M. Ceriotti, *A data-driven interpretation of the stability of organic molecular crystals*, Chemical Science (2022), doi:10.1039/D2SC06198H.
- [3] G. Fraux, R. Cersonsky, and M. Ceriotti, *Chemiscope: interactive structure-property explorer for materials and molecules*, Journal of Open Source Software **5**, 2117 (2020).
- [4] M. J. Willatt, F. Musil, and M. Ceriotti, *Feature Optimization for Atomistic Machine Learning Yields a Data-Driven Construction of the Periodic Table of the Elements*, Physical Chemistry Chemical Physics **20**, 29661 (2018).
- [5] J. Nigam, M. J. Willatt, and M. Ceriotti, *Equivariant representations for molecular Hamiltonians and N-center atomic-scale properties*, The Journal of Chemical Physics **156**, 014115 (2022).
- [6] 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).
- [7] A. Fabrizio, A. Grisafi, B. Meyer, M. Ceriotti, and C. Corminboeuf, *Electron density learning of non-covalent systems*, Chemical Science **10**, 9424 (2019).
- [8] C. B. Mahmoud, F. Grasselli, and M. Ceriotti, *Predicting hot-electron free energies from ground-state data*, Physical Review B **106**, L121116 (2022).
- [9] 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).
- [10] A. Fabrizio, K. R. Briling, and C. Corminboeuf, *SPA^{H}M: the spectrum of approximated Hamiltonian matrices representations*, Digital Discovery **1**, 286 (2022).
- [11] F. Musil, M. Veit, A. Goscinski, G. Fraux, M. J. Willatt, M. Stricker, T. Junge, and M. Ceriotti, *Efficient implementation of atom-density representations*, The Journal of Chemical Physics **154**, 114109 (2021).
- [12] A. Grisafi and M. Ceriotti, *Incorporating long-range physics in atomic-scale machine learning*, The Journal of Chemical Physics **151**, 204105 (2019).
- [13] S. Vela, R. Laplaza, Y. Cho, and C. Corminboeuf, *cell2mol: encoding chemistry to interpret crystallographic data*, npj Computational Materials **8**, 188 (2022).
- [14] S. Gallarati, P. van Gerwen, R. Laplaza, S. Vela, A. Fabrizio, and C. Corminboeuf, *OSCAR: an extensive repository of chemically and functionally diverse organocatalysts*, Chemical Science **13**, 13782 (2022).
- [15] S. Gallarati, P. van Gerwen, R. Laplaza, S. Vela, A. Fabrizio, and C. Corminboeuf, *OSCAR: An extensive repository of chemically and functionally diverse organocatalysts*, Materials Cloud Archive **2022.106** (2022), doi:10.24435/materialscloud:v4-sn.
- [16] G. Imbalzano, Y. Zhuang, V. Kapil, K. Rossi, E. A. Engel, F. Grasselli, and M. Ceriotti, *Uncertainty estimation for molecular dynamics and sampling*, The Journal of Chemical Physics **154**, 074102 (2021).
- [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).

List of year 9 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).

⬢○ 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).
Group(s): Ceriotti, Marzari, Pizzi / Project(s): P2, P3, P4
Related datasets: doi.org/10.24435/materialscloud:9g-k6

⬢○ M. Ceriotti
Beyond Potentials: Integrated Machine Learning Models for Materials
MRS Bulletin **47** (2022).
Group(s): Ceriotti / Project(s): P2
Related datasets: not applicable

⬢○ R. Fabregat, A. Fabrizio, E. A. Engel, B. Meyer, V. Juraskova, M. Ceriotti, and C. Corminboeuf
Local kernel regression and neural network approaches to the conformational landscapes of oligopeptides
Journal of Chemical Theory and Computation **18**, 1467 (2022).
Group(s): Ceriotti, Corminboeuf / Project(s): P2
Related datasets: doi.org/10.5281/zenodo.5172582

○ C. B. Mahmoud, F. Grasselli, and M. Ceriotti
Predicting hot-electron free energies from ground-state data
Physical Review B **106**, L121116 (2022).
Group(s): Ceriotti / Project(s): P2
Related datasets: doi.org/10.24435/materialscloud:36-ff

⬢○ B. A. Helfrecht, G. Pireddu, R. Semino, S. M. Auerbach, and M. Ceriotti
Ranking the Synthesizability of Hypothetical Zeolites with the Sorting Hat
Digital Discovery **1**, 779 (2022).
Group(s): Ceriotti / Project(s): P2
Related datasets: doi.org/10.24435/materialscloud:xw-5k

○ H. J. Kulik, T. Hammerschmidt, J. Schmidt, S. Botti, M. A. L. Marques, M. Boley, M. Scheffler, M. Todorović, P. Rinke, C. Oses, A. Smolyanyuk, S. Curtarolo, A. Tkatchenko, A. P. Bartók, S. Manzhos, M. Ihara, T. Carrington, J. Behler, O. Isayev, M. Veit, A. Grisafi, J. Nigam, M. Ceriotti, K. T. Schütt, J. Westermayr, M. Gastegger, R. J. Maurer, B. Kalita, K. Burke, R. Nagai, R. Akashi, O. Sugino, J. Hermann, F. Noé, S. Pilati, C. Draxl, M. Kuban, S. Rigamonti, M. Scheidgen, M. Esters, D. Hicks, C. Toher, P. V. Balachandran, I. Tamblyn, S. Whitelam, C. Bellinger, and L. M. Ghiringhelli
Roadmap on Machine Learning in Electronic Structure
Electronic Structure **4**, 023004 (2022).
Group(s): Ceriotti / Project(s): P2
Related datasets: not applicable

⬢○ J. Nigam, S. Pozdnyakov, G. Fraux, and M. Ceriotti
Unified Theory of Atom-Centered Representations and Message-Passing Machine-Learning Schemes
The Journal of Chemical Physics **156**, 204115 (2022).
Group(s): Ceriotti / Project(s): P2
Related datasets: doi.org/10.24435/materialscloud:3f-g3

○ 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).
Group(s): Ceriotti / Project(s): P2
Related datasets: not applicable

⬢○ R. K. Cersonsky, M. Pakhnova, E. A. Engel, and M. Ceriotti
A data-driven interpretation of the stability of organic molecular crystals
Chemical Science (2022), doi:10.1039/D2SC06198H.
Group(s): Ceriotti / Project(s): P2
Related datasets: doi.org/10.24435/materialscloud:71-21

⬢○ A. Fabrizio, K. R. Briling, and C. Corminboeuf
SPA^{H}M: the spectrum of approximated Hamiltonian matrices representations
Digital Discovery **1**, 286 (2022).
Group(s): Corminboeuf / Project(s): P2
Related datasets: doi.org/10.24435/materialscloud:js-pz

S. Vela, R. Laplaza, Y. Cho, and C. Corminboeuf
cell2mol: encoding chemistry to interpret crystallographic data
npj Computational Materials **8**, 188 (2022).
Group(s): Corminboeuf / Project(s): P2
Related datasets: doi.org/10.24435/materialscloud:g5-5r

S. Gallarati, P. van Gerwen, R. Laplaza, S. Vela, A. Fabrizio, and C. Corminboeuf
OSCAR: an extensive repository of chemically and functionally diverse organocatalysts
Chemical Science **13**, 13782 (2022).
Group(s): Corminboeuf / Project(s): P2
Related datasets: doi.org/10.24435/materialscloud:v4-sn

P. van Gerwen, A. Fabrizio, M. Wodrich, and C. Corminboeuf
Physics-based representations for machine learning properties of chemical reactions
Machine Learning: Science and Technology **3**, 045005 (2022).
Group(s): Corminboeuf / Project(s): P2
Related datasets: doi.org/10.5281/zenodo.6627913

Pillar 3 — Digital Infrastructure of Open Simulations and Data

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

Partner: Sara Bonella (EPFL)

1 Progress of the different efforts

1.1 AiiDA

AiiDA 2.0, 2.1 and 2.2 were released in year 9, with substantial improvements to the data storage and archival design to support pre-exascale projects. The storage size of an AiiDA project is reduced by up to 80% via compression and de-duplication of millions of files, and their packing into a minimal number of large binary objects. This design, inspired by Git's internal design, allows for efficient storage and backup of data, whilst still maintaining optimal concurrent read/write access.

To show AiiDA's ability to run on pre-exascale machines, we obtained exclusive access to the CPU partition of the new LUMI supercomputer, where we used AiiDA to orchestrate 55'704 QUANTUM ESPRESSO calculations in $\sim$ 14 hours, optimizing the geometry of 15'324 compounds. Using the error recovery features implemented in the AiiDA QUANTUM ESPRESSO workflows, 7'887 issues were dealt with on the fly without any user intervention. Fig. 1 shows the usage of the LUMI CPU partition during our "hero run", clearly demonstrating that after an initial startup period, AiiDA can continuously fill the pre-exascale machine without any issue.

In parallel, the AiiDA ecosystem continues to grow, currently with 83 plugin packages and 117 workflows on the AiiDA plugin registry[1]. For the QUANTUM ESPRESSO plugin package in particular, developed by MARVEL, there are now robust workflows to calculate geometry optimization, band structure and projected density of stated (PDOS). Protocols have been developed for these fundamental workflows, providing a set of rigorously tested input parameters without requiring extensive knowledge on the code. This is essential to make them available as turnkey workflows through AiiDAlab (see Section 1.4). Further developments focused on the phonon code of QUANTUM ESPRESSO, with new workflows for calculating the dynamical matrix, phonon dispersion [1, 2] (Fig. 2) and electron-phonon coupling.

To simplify running workflows calculating a certain material property across various codes, we developed a common interface for running a geometry optimization [3], currently supporting 13 quantum engines. Via this common interface we can design higher-level code-agnostic work chains, i.e. a single implementation that can run via any of the supported quantum engines. This common workflow is being currently used in a large collaborative

[1] https://aiidateam.github.io/aiida-registry/

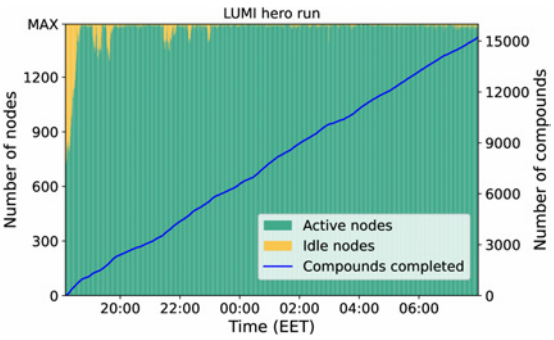


Figure 1: *"Hero run" on the full LUMI-C supercomputer: AiiDA was able to completely fill the whole machine, computing 15'324 compounds in 14 hours.*

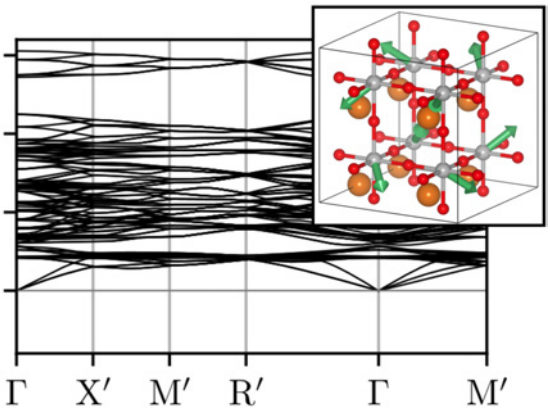


Figure 2: *Phonon dispersion of the 40-atom prototype of cubic $BaTiO_3$ with all phonons real and positive [1], calculated with the recently developed* `PhononDispersionWorkChain` *for AiiDA.*

verification project studying a set of 960 unary and oxide structures for 96 elements, and proving very valuable to check results consistency across codes, leading to the improvement of protocols and pseudopotential sets used.

1.2 Materials Cloud

Materials Cloud continues to be widely used within the materials science community, attracting over 15k unique monthly visits as of November 2022. Each of the five sections — *Learn*, *Work*, *Discover*, *Explore* and *Archive* — continue to expand with new additions.

The *Archive*, our open-access and moderated research data repository, is now recommended also by SNSF (in addition to the *Nature*'s *Scientific Data* and EU Commission's *Open Research Europe* journals), and it includes 734 published records as of December 2022, with over 29 million crystal structures contained in these entries. The number of new registered users in 2022 was over 240, reaching a total of 773 users. *Archive* entries that contain AiiDA files can be directly explored using the Renku platform[2] and datasets compatible with chemiscope can be directly visualized via the corresponding tool[3]. Planning for the migration to the latest long-term support release of InvenioRDM[4] are ongoing, bringing the benefits of a more modern and user-friendly interface, combined with improved interoperability with external apps.

The *Discover* section of Materials Cloud has grown to host 16 highly curated datasets, with latest additions including "Pyrene-based metal organic frameworks", "Molecule vibration explorer" and "Donor-acceptor copolymers for intramolecular singlet fission". Additionally, new data contributions to the Materials Cloud 2D crystals database (MC2D) were added [4]. The corresponding *Explore* sections for AiiDA datasets were also updated: as a whole, the *Explore* section now contains 3.9 million data and calculation nodes with full AiiDA provenance.

A web application was developed to explore the results of the AiiDA common workflows verification project, mentioned in Section. 1.1 (Fig. 3). The application is already temporarily available online[5] and will be published as a Materials Cloud *Discover* section upon publication of the corresponding paper.

The list of scientific tools in the Materials Cloud *Work* section now includes 13 entries. The latest additions include the "Twisted mixed multilayer graphene in the k·p model" and "Machine-learning accelerated identification of exfoliable two-dimensional materials" [5].

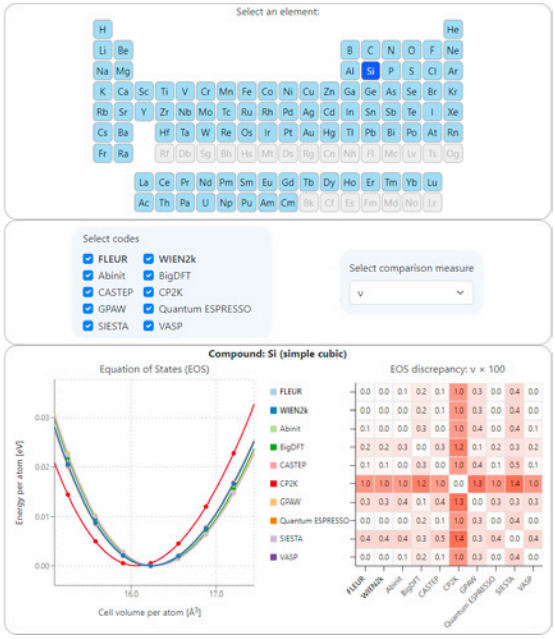


Figure 3: *Web app to explore and compare equation-of-state (EoS) calculations performed with the AiiDA common workflows for 10 DFT packages. The user can select an element, which software packages to compare, and a comparison measure; the EoS curves together with a comparison matrix for the chosen measure are displayed for all structures (unaries and oxides) containing the selected element.*

The *Learn* section of Materials Cloud has expanded to include over 200 recordings of lectures, discussions and tutorial sessions. Considerable effort has been put toward building the novel Lhumos educational portal discussed in the next paragraph, as its future replacement.

1.3 Lhumos

The Learning Hub for Modelling and Simulation (Lhumos) platform is a collaboration between MARVEL, CECAM, and MaX and aims at developing a bespoke web portal to collect and disseminate basic and advanced material for continuous training, with particular focus on materials simulations. It will contain videos, lecture notes, links to Git repositories of codes and tutorials, enabling researchers and students to access state-of-the-art training material. It will also provide a hub for institutions or projects that wish to contribute to this community-driven repository. An overview of the platform is shown in Fig. 4. Lhumos combines the Clowder framework to store the

[2] https://renkulab.io/
[3] https://chemiscope.org/
[4] https://inveniordm.docs.cern.ch/
[5] https://acwf-verification.materialscloud.org

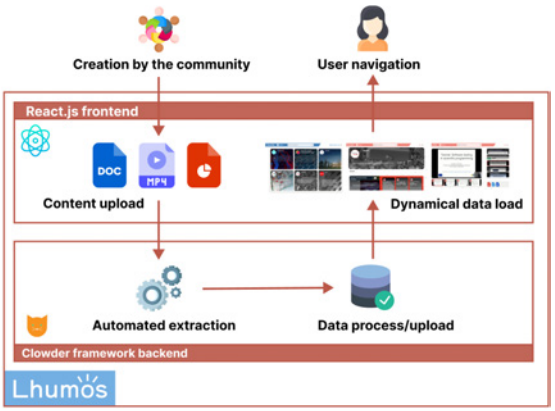


Figure 4: *Overview of the Lhumos platform..*

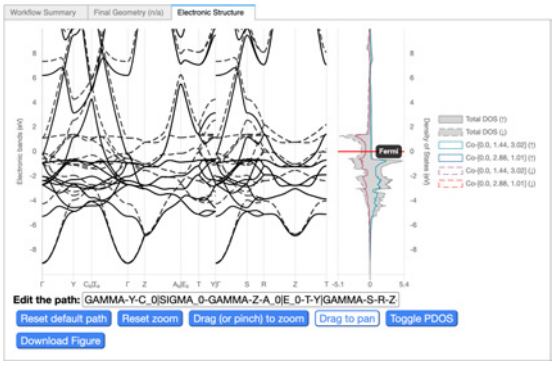


Figure 5: *Band structure and PDOS of Cobalt, calculated with the AiiDAlab* QUANTUM ESPRESSO *app.*

material, with a custom designed frontend for user access, that we develop in React.js. Key design concepts are: easy access, intuitive content navigation, fast searches, automation of uploaded video processing, and a flexible design enabling to retain specific visual identities (e.g., of projects) while profiting of the increased visibility of a single entry point shared with other relevant partners. A full time human resource (Roberto Bendinelli), hired at EPFL since Nov 2021, develops the portal. Funding for this position was shared, in the first year, by MaX, CECAM and MARVEL and now continues with 50% funding from MARVEL and 50% from CECAM. In year 9, we updated and deployed the Clowder framework on CSCS, we planned and developed key parts of the Lhumos web frontend, and we developed and tested bespoke APIs for seamless communication between the Clowder repository and the web frontend, with minimal bandwidth requirements. Deployment of a beta version of Lhumos is planned for the first quarter of 2023.

1.4 AiiDAlab

We have created instructions and templates to deploy custom AiiDAlab instances on Kubernetes, and on Azure cloud resources in particular[6]. The latter makes AiiDAlab able to run HPC calculations within Azure without additional supercomputing resources. The team also provided support for the deployment of AiiDAlab instances to EU projects (such as the H2020 Materials Modeling MarketPlace) and companies (a representative of Sandvik Coromant via the public mailing list). We also developed the aiidalab-launch[7] tool, enabling users to launch an AiiDAlab instance directly on their local computer across all major operating systems. The computer and code setting procedures in the apps were refactored, simplifying configuration. The aiida-code-registry[8] was created and acts as a centralized database of configuration templates for computational clusters. The QUANTUM ESPRESSO app was updated with a new bands widget (Fig. 5), which displays interactively high-quality band structure and projected density of stated (PDOS), supporting also magnetic materials.

A new "Molecules" app was developed at Empa to compute electronic properties of small molecules (such as ionization potential, excitation energy, natural orbitals, and more) using the Gaussian code. A second new app developed at EPFL is the "SSSP pseudopotential toolkit". It runs complex workflows to verify the quality of pseudopotentials, providing also tools to compare them and identify converged numerical parameters for simulations.

1.5 Quantum Mobile

The Quantum Mobile virtual machine has expanded to incorporate updated versions of relevant quantum simulation codes, including Abinit, BIGDFT, CP2K, NWChem, FLEUR, QUANTUM ESPRESSO, SIESTA, Yambo, and Wannier90. All codes are integrated with the AiiDA engine, to provide a comprehensive and standardized environment for delivering hands-on teaching[9]. This has been used to deliver various tutorials, including the recent "Advanced QUANTUM ESPRESSO: Hubbard and Koopmans functionals from linear response" in November 2022. To facilitate accelerated release cycles and ease of main-

[6] https://github.com/aiidalab/aiidalab-on-azure
[7] https://github.com/aiidalab/aiidalab-launch
[8] https://github.com/aiidalab/aiida-code-registry
[9] https://sites.google.com/view/hubbard-koopmans/quantum-mobile

tenance, deployment of individual codes has been moved to the open-source conda-forge[10] package manager, where all MARVEL codes are now available, allowing users to also easily install them on their local machines within isolated environments.

1.6 SIRIUS and MaZe

In year 9, SIRIUS has been successfully ported to the AMD GPU architecture, with a complete native (ROCm) port developed in close collaboration with AMD engineers (SIRIUS was one of the early adopters of the ROCm BLAS/LAPACK stack). SIRIUS is now fully functional on AMD Mi250, and thus LUMI. One node of LUMI outperforms 8 nodes of Piz Daint by $2-3\times$, depending on the system. As a result, the Marzari group was able to get access to the LUMI Pilot phase, and won a significant ($>$ 1 M GPU h) grant on LUMI via the Swiss (CSCS) Chronos track. Similarly, the Ceriotti group was able to submit a proposal for the EuroHPC extreme scale call.

SIRIUS also gained wider integration in community codes, including QUANTUM ESPRESSO, CP2K, BIGDFT, and Exciting. The latter three codes integrated SIRIUS in their main branches, the integration in QUANTUM ESPRESSO is maintained in a separate repository. With spack, installation is as easy as `spack install q-e-sirius ^sirius+cuda`. The integration in Exciting has been finalized in year 9, while the other integrations have been maintained (e.g. version upgrades) in the same period.

The direct minimizer based on non-linear conjugate-gradients (NLCG) has been finalized and is now of production quality. For the case of norm-conserving pseudopotentials, it shows a 100% success rate. For ultrasoft pseudopotentials, the success rate depends on the element type, being $\sim$ 80% for the most difficult class (lanthanides), and approaching 100% when lanthanides are not included (Fig. 6).

Finally, preparatory work necessary for the integration of Mass Zero (MaZe) first-principles dynamics in SIRIUS, foreseen for year 10, was completed. In particular the generalization of the formalism from orbital-free to Kohn-Sham DFT has been developed, and a MARVEL-funded PhD student (Edrick Solis Gonzales) was hired in November 2022.

[10] https://conda-forge.org/

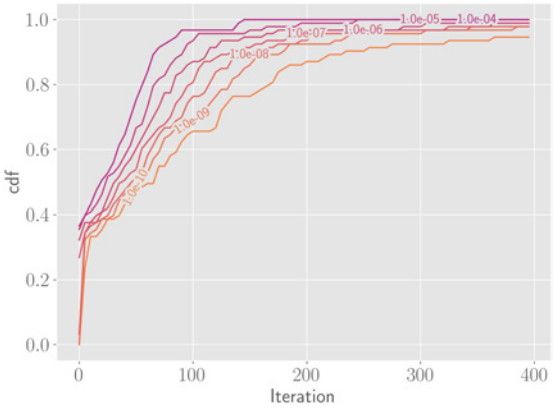


Figure 6: *Convergence benchmarks for 100 structures not containing lanthanides which failed to converge with standard SCF, showing the percentage of structures converged to a given tolerance within a given number of CG steps. We used the more challenging ultrasoft/PAW pseudopotentials from SSSP, with a success rate approaching 100% (for norm-conserving pseudos, we obtain a 100% success rate).*

2 Contribution to overall goals and initial proposal

Significant progress was made towards the key goals of Pillar 3, namely of preparing for the exascale challenge (both in terms of robustness and scalability), making all codes and algorithms widely usable also by non-experts, and delivering a self-sustaining long-term infrastructure for simulations. All these progresses ultimately contribute to MARVEL's goal of accelerated design and discovery of materials via a materials informatics platform of high-throughput simulations, verified thanks to code interoperability.

Indeed, the effectiveness of AiiDA's redesign for improved scalability was demonstrated during the "hero run" on LUMI-C. Improved robustness is achieved both through error recovery features in AiiDA workflows and the new ensemble-DFT minimizer in SIRIUS. Thanks to SIRIUS's support for new GPU architectures, our workflows can be run on the latest pre-exascale machines, including the AMD GPU partition of LUMI. Moreover, protocols have been developed to run the workflows in high throughput, and verified comparing results across codes via the common workflow interface. These workflows will be made available to non-experts via AiiDAlab, now much easier to deploy both on local machines and on the cloud. Together with Quantum Mobile for tutorials, MARVEL Pillar 3 offers a broad range of solutions for running advanced materials simulations with minimal setup. Once obtained, results can be then seam-

lessly shared on Materials Cloud, whose user base continues to expand across all sections. On top of the education resources in the Materials Cloud *Learn* section, the new Lhumos platform is being developed as a long-term, community-driven repository of tutorial material for materials simulations.

3 Collaborative and interdisciplinary components

The development of the ensemble-DFT algorithm in the SIRIUS code at CSCS has been rigorously tested by the AiiDA team at EPFL, with an ongoing collaboration to integrate them. Many contributions to the Materials Cloud *Discover* and *Work* sections were provided by other MARVEL groups. In addition, the new Lhumos portal is being collaboratively developed by MARVEL, CECAM and MaX. Furthermore, efforts for education as interactive scientific visualizations continue to develop in collaboration with the OSSCAR project at EPFL [6].
Tight collaborations continue also at the European level with large TIER-0 HPC centers in Europe, with the Battery2030+ project BIG-MAP, with many H2020 projects (the MaX and TREX CoE, Marketplace, Intersect, Dome 4.0, OpenModel). We expect tight collaboration also with the new ORD-R Establish project "PREMISE" recently funded by the ETH Domain, adopting AiiDA as a reference workflow engine for simulations (and openBIS as an electronic lab notebook (ELN) for experiments), towards providing standard approaches and metadata formats to facilitate FAIR data exchange between simulations and experiments in materials science. Many international collaborations are also ongoing for the development of codes and workflows, e.g. with SINTEF Norway (VASP), Microsoft (AiiDA, AiiDAlab), or University of Parma, Italy (muon spectroscopy via QUANTUM ESPRESSO).

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. Kotiuga, S. Halilov, B. Kozinsky, M. Fornari, N. Marzari, and G. Pizzi, *Microscopic picture of paraelectric perovskites from structural prototypes*, Physical Review Research **4**, L012042 (2022).
- [2] 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).
- [3] S. P. Huber, E. Bosoni, M. Bercx, J. Bröder, A. Degomme, V. Dikan, K. Eimre, E. Flage-Larsen, A. Garcia, L. Genovese, D. Gresch, C. Johnston, G. Petretto, S. Poncé, G.-M. Rignanese, C. J. Sewell, B. Smit, V. Tseplyaev, M. Uhrin, D. Wortmann, A. V. Yakutovich, A. Zadoks, P. Zarabadi-Poor, B. Zhu, N. Marzari, and G. Pizzi, *Common workflows for computing material properties using different quantum engines*, npj Computational Materials **7**, 136 (2021).
- [4] D. Campi, N. Mounet, M. Gibertini, G. Pizzi, and N. Marzari, *Novel materials in the Materials Cloud 2D database*, arXiv:2210.11301 (2022).
- [5] M. T. Vahdat, K. V. Agrawal, and G. Pizzi, *Machine-learning accelerated identification of exfoliable two-dimensional materials*, Machine Learning: Science and Technology **3**, 045014 (2022).
- [6] D. Du, T. J. Baird, S. Bonella, and G. Pizzi, *OSSCAR, an Open Platform for Collaborative Development of Computational Tools for Education in Science*, Computer Physics Communications **282**, 108546 (2023).

List of year 9 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).

⬢○ M. KOTIUGA, S. HALILOV, B. KOZINSKY, M. FORNARI, N. MARZARI, AND G. PIZZI
Microscopic picture of paraelectric perovskites from structural prototypes
Physical Review Research **4**, L012042 (2022).
Group(s): Marzari, Pizzi / Project(s): P3,P4,OSP
Related datasets: doi.org/10.24435/materialscloud:jc-ky

⬢○ 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).
Group(s): Ceriotti, Marzari, Pizzi / Project(s): P2, P3, P4
Related datasets: doi.org/10.24435/materialscloud:9g-k6

⬢○ M. T. VAHDAT, K. V. AGRAWAL, AND G. PIZZI
Machine-learning accelerated identification of exfoliable two-dimensional materials
Machine Learning: Science and Technology **3**, 045014 (2022).
Group(s): Pizzi / Project(s): P3
Related datasets: doi.org/10.24435/materialscloud:m4-7f

D. Du, T. J. Baird, S. Bonella, and G. Pizzi
OSSCAR, an Open Platform for Collaborative Development of Computational Tools for Education in Science
Computer Physics Communications **282**, 108546 (2023).
Group(s): Bonella, Pizzi / Project(s): P3
Related datasets: doi.org/10.17632/26py5zz9f8.1

D. Campi, N. Mounet, M. Gibertini, G. Pizzi, and N. Marzari
Novel materials in the Materials Cloud 2D database
arXiv:2210.11301 (2022).
Group(s): Marzari, Pizzi / Project(s): P3, P4, DD3
Related datasets: doi.org/10.24435/materialscloud:36-nd

Pillar 4

Long-term Integration in the Swiss Scientific Landscape

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

1 Progress of the different efforts

The goal of Pillar 4 is to plan, deploy, and ultimately phase-in the post-2026 embedding of MARVEL in the Swiss scientific landscape, in the form of core partnerships with PSI and Empa. In July 2021, PSI has created an entire new Division dedicated to Scientific Computing, Theory and Data, directed by Prof. Christian Rüegg, with a number of scientific and technical laboratories. These include the Laboratory for Materials Simulations developed in close partnership with MARVEL, and headed by Prof. Nicola Marzari (thanks to a temporary 20% appointment at PSI), and comprising three groups: one on Materials Software and Data, with an initial planning for 6 scientists (3 tenure-track, 3 postdocs), dedicated to expanding further the simulation capabilities for the prediction and characterization of materials properties; one on Multiscale Materials Modelling, led by Dr. Matthias Krack, and a third one on Light-Matter Interactions, where a new PATT joint by UniFR and PSI will be located, and also supported with one PhD student from MARVEL. Dr. Giovanni Pizzi has been hired, from Feb 2022, as group leader for the Materials Software and Data group, and Prof. Michael Schüler, from Jan 2022, as group leader for the Light-Matter Interactions group. All the efforts from MARVEL are cash matched both by PSI and by Empa

1.1 PSI: Computational spectroscopies

The goals for the 4 years of phase III are to push the development of vibrational spectroscopies (IR and Raman), angle-resolved photoemission spectroscopy (ARPES), X-ray absorption (XAS) and resonant-inelastic X-ray scattering (RIXS), model Hamiltonians for magnetic materials, muon rest sites, and ultrafast dynamics (this latter, of competence of the new UniFR/PSI PATT), all of these based on state-of-the-art functionals for ground states (Koopmans functionals) and excited states (Hubbard functionals)

a) *Koopmans functionals* Koopmans spectral functionals have been proven to be able to simultaneously and accurately describe ground state properties and charged excitations of atoms, molecules, nanostructures [1] and periodic crystals [2]. During year 1 of phase III we have been working on two complementary solutions toward an efficient, consistent, and user friendly implementation and deployment of Koopmans' spectral functionals: on one side we have developed a novel implementation for periodic systems (but also readily applicable to finite ones) using maximally localized Wannier functions (MLWF) and a linear response approach to compute the screened Koopmans corrections. The resulting code is named KCW [3] and, at variance with the original implementation, does not require the use of expensive supercell calculations. KCW is an open-source software distributed under the terms of the GPL as a component of QUANTUM ESPRESSO (QE) package since the official release 7.1 (June 2022). KCW provides an interface with the PWscf package of QE and Wannier90, two open-source and widely used electronic structure tools. On the other side, we have automated and strengthened the original, and more general, supercell implementation based on a finite difference approach for the evaluation of screened Koopmans corrections. To this end we have developed an open-source python package `koopmans` based on the atomistic simulation environment [11] that automates the process of performing a Koopmans calculation from start to finish. Both the supercell and primitive cell implementations are supported and it is simple to switch from one to the other. This code allows the user to perform Koopmans calculations in a robust, automated, and user-friendly fashion that does not require expert knowledge. The entire code base was released publicly in mid-2022[1] with an accompanying website for documentation and dissemination[2].

b) *Extended Hubbard functionals* Key ingredient for reliable density-functional theory (DFT) calculations is the availability of accurate exchange-correlations functionals. Extended

[1] https://github.com/epfl-theos/koopmans
[2] https://koopmans-functionals.org

Hubbard functionals (DFT+U+V) have proven to be one of the most accurate ones for modeling complex transitional-metal compounds such as those used as cathodes in Li-ion batteries [4]. During year 1 of phase III we have delivered the HP code [5] distributed with QUANTUM ESPRESSO for computing Hubbard parameters based on density-functional perturbation theory [6]. The HP code does not require the use of computationally expensive supercells of the traditional linear-response approach; instead, unit cells are used with monochromatic perturbations that significantly reduce the computational cost of determining Hubbard parameters. HP is an open-source software distributed under the terms of the GPL as a component of QUANTUM ESPRESSO. As with other components, HP is optimized to run on a variety of different platforms, from laptops to massively parallel architectures, using native mathematical libraries (LAPACK and FFTW) and a hierarchy of custom parallelization layers built on top of MPI. This is the base for spectroscopic calculations described below.

c) *X-ray absorption and photoelectron spectroscopies (XAS and XPS)* XAS and XPS are the core-electron-excitation techniques that are used to probe the empty and occupied electronic states of materials, respectively. During year 1 of phase III, we have been developing a computational setup for the calculation of the XAS and XPS spectra (K edge) based on the Fermi's golden rule. This is handled by several steps: (i) ground-state DFT calculation without a core hole, (ii) determination of the symmetry-inequivalent atoms, (iii) ground-state calculations with a core hole using large supercells and pseudopotentials generated with the core hole, (iv) calculation of the core-electron binding energies to determine the chemical shifts, (v) calculation of the matrix elements describing core-electron excitations, (vi) plot of the XPS and XAS spectra. We have already started to implement the AiiDA workflows for the above calculations. The goal is to have robust workflows that provide base spectrum calculation as well as handle the advanced setup for various materials (e.g. crystal and powder samples). The workflows will allow the integration of the XAS and XPS calculations with the AiiDAlab platform to provide a user-friendly GUI for experimental collaborators.

d) *Vibrational spectroscopies* Raman spectroscopy is nowadays a ubiquitous method used in every experimental laboratory for materials characterization. Nevertheless, interpretation of such spectra is more than often a difficult task to carry out, and theoretical support is desired. DFT+U+V can be employed to reliably assign the observed peaks to microscopic structural features. During year 1 of phase III, we have developed a user-friendly AiiDA workflow [7] that allows to run a full vibrational spectra simulation specifying only three inputs: the structure, the protocol (a string describing in a general way the desired accuracy) and the code (i.e., where to run the calculations). The workflow exploits the finite displacements and finite fields method [12] to compute the needed tensorial components for the phonon and the intensities, respectively. The methodology allows for the one-shot calculation of mixed third order derivatives in electric fields through the finite differentiation of forces and polarization, and requires at most only 13 self-consistent field runs, not depending on the symmetry of the system. Furthermore, such method can be employed straight away with extended Hubbard functionals. In Fig. 1 we show the DFT+U+V Raman spectra of $FePO_4$ (a delithiated Li-ion battery cathode material) in comparison with the experiments. As can be see, the agreement with the experimental measurements is very good.

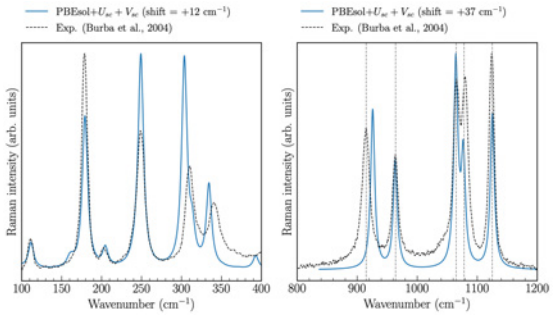


Figure 1: *Comparison of the computed and experimental Raman spectra for $FePO_4$. DFT+U+V calculations were performed using the PBEsol functional and self-consistent Hubbard parameters U_{sc} and V_{sc} determined using the HP code of* QUANTUM ESPRESSO. *All calculations were handled using AiiDA.*

1.2 AiiDAlab

Phase III at Empa started with hiring Aliaksandr Yakutovich as a scientist to support the core development of AiiDAlab for the continued evolution of the platform and the further development of apps to support combined computational experimental research. Starting in November 2022 an additional postDoc, Andres Ortega-Guerrero is working on the goals

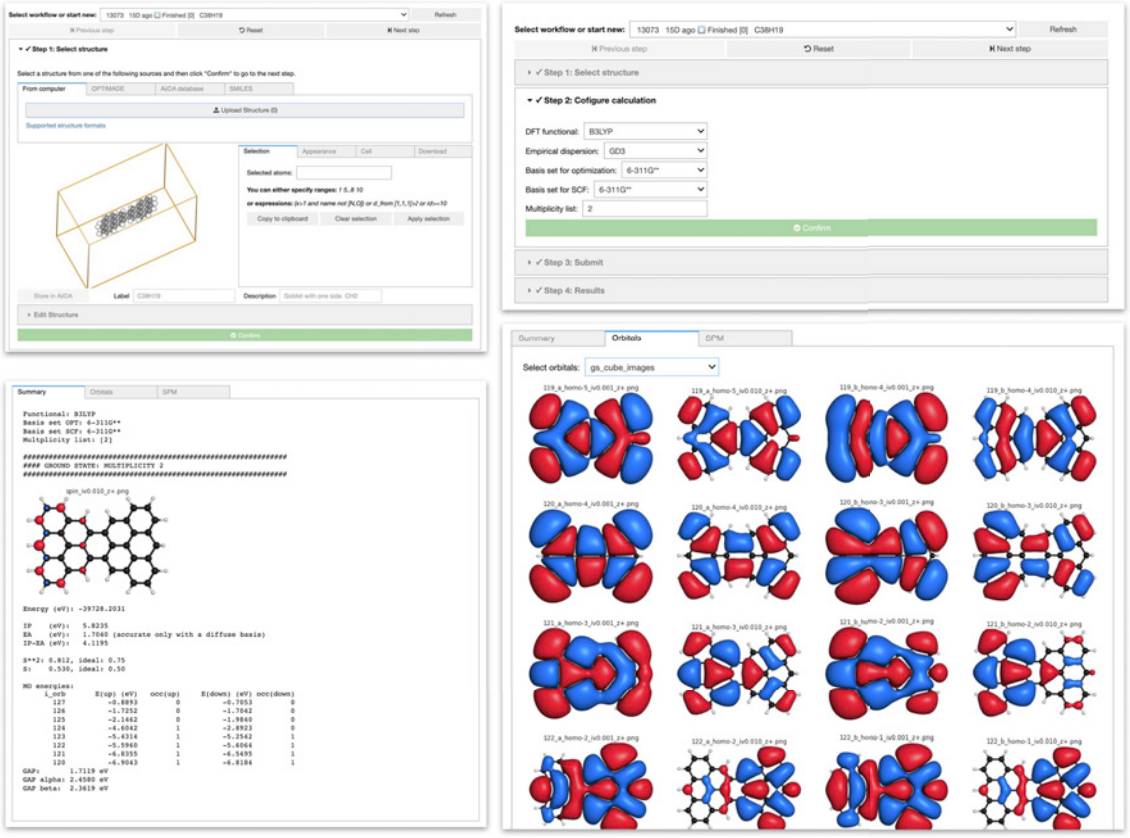


Figure 2: *The screenshots in this image show different steps of the "Molecules" app. In the top left panel, the user provides the initial structure that could be uploaded, for example, from an open-access repository via the "OPTIMADE" tab. Once the structure is selected, the user can modify it using the integrated structure editor. In the top right panel, the user selects the DFT functional, dispersion interaction corrections, basis set, and multiplicities. The lower panels show a summary of the computed quantities and the computed orbitals.*

of Pillar 4. The continued support to experimentalists with the AiiDAlab platform resulted in publications of scientific work related to on-surface chemistry that spans from unravelling intriguing diradical aspects in heteroatom substituted acenes [8] up to fabrication of novel carbon-based 1D nanomaterials where we highlight new synthesis routes for polyarylenes by cycloaromatization of isopropyl substituents [9]. Also worth mentioning is our recent work to understand the role of Au adatoms in the polymerization process for the on-surface synthesis of carbon-based nanostructures [10].

For the development of the AiiDAlab core crucial was the work done by the AiiDAlab team (in collaboration with Pillar 3). To increase the team productivity we synchronized the code styling and automated release processes for all the core AiiDAlab packages. We also keep adding more tests to increase the stability of the AiiDAlab infrastructure. We continue adding more tools and widgets to empower app developers for creating better apps. For instance, we created an all-in-one computational resources widget that allows to select and to setup computational resources all in one place. For easy crystal structure handling, we added a cell editor allowing for easy cell manipulations. Our automatically build AiiDAlab docker stack has been redesigned using the official Jupyter image as the base. Until recently, the PostgreSQL (core dependency of AiiDA) database migration had to be done manually. With the new update, we implement a fully automated migration. To enhance user experience we implemented an "open app" tool that lets a user quickly install a requested application if it is not yet available in AiiDAlab. Finally, AiiDAlab and all the apps in the registry have been migrated to provide full support for AiiDA 2.0 functionality.

We had a request from the experimental collaborators in the nanotech@surfaces laboratory for the development of an application to efficiently characterize spin states in magnetic nanocarbons. This resulted in the creation of the "Molecules" AiiDAlab application. The app

relies on the workflows implemented within aiida-nanotech-empa package[3]. The first step of the workflow is the geometry optimization of the structure. This is done for each individual multiplicity provided by the user. The total energies of optimized structures with different multiplicities are then compared and the combination structure-multiplicity with the lowest energy is further referred to as the ground state. Once the optimized geometries for each multiplicity are obtained, the next step is to perform a separate self-consistent field (SCF) run followed by the cube file generation. Those cube files are further displayed in the app (Fig. 2). The ground state structure is used to compute the fundamental gap as the difference between the ionization potential and the electron affinity. Spin excitation energies are also reported.

We already started collaborations with different Empa laboratories to explore the application of MARVEL solutions to fields outside of materials science. For atmospheric simulations, we started a collaboration with the Pizzi group (Pillar 3) and the Laboratory of Atmospheric Modelling and Remote Sensing at Empa (Stephan Henne). The laboratory develops and applies a suite of atmospheric transport models and inverse modeling tools. Both Lagrangian particle dispersion models (LPDMs), as well as Eulerian models (extensions to typical weather prediction models), are used. These systems are applied to estimate the emissions of greenhouse gases into the atmosphere based on observations of atmospheric concentrations (*in situ* or remote sensing).

Our collaboration allowed releasing the AiiDA plugin for the FLEXPART-COSMO code, which is used by a large community. In the field of atmospheric modeling, it is common to keep input data in long-term storage (like tape) due to their large size. Herein, the data copying from the tape to the scratch folder is typically the first step of the workflow. Further, a FLEXPART-COSMO simulation is run using those files as input. The simulation typically runs in parallel for multiple locations and multiple time frames. The output data produced by the workflow are further used for post-processing. The selected post-processed data are then transferred back to tape for long-term storage. In case of issues with simulations, the workflow enters the restart loop trying to handle the encountered errors and restarting the simulations with modified inputs. The scheme shown in Fig. 3 is an example of AiiDA plugins

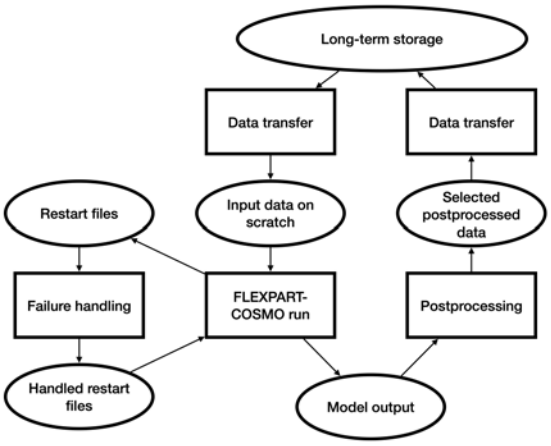


Figure 3: *The figure depicts the FLEXPART-COSMO simulation workflow. The starting point is the extraction of data from long-term storage. Further, the data is used as input for the FLEXPART-COSMO simulations, which typically run for multiple locations in parallel. In case of simulation issues, the restart handler tries to fix them and reruns the workflow. The simulated data are further post-processed and transferred back on tape for long-term storage*

and workflows to automate the typical tasks and processing steps encountered in regional-scale inverse modeling of atmospheric trace species such as greenhouse gases. This first effort triggered new collaborative work that allowed us to obtain additional funds through the ORD-R measure of the ETH board.

Collaboration with Giovanni Pizzi and Empa scientific IT allowed starting the search for solutions to integrate AiiDAlab with electronic laboratory notebook (ELN) and laboratory information management systems. In Fig. 4 we show an example where starting from an inventory of chemicals in the openBIS ELN, we can start simulations in AiiDAlab and migrate the results back to the ELN. Also this effort triggered collaborative projects with the ETHZ-SIS group responsible for the openBIS ELN-LIMS platform, Pillar 3 at PSI, and the Laboratory Materials for Energy Conversion at Empa.

2 Contribution to overall goals and initial proposal

This project is fully in sync with the overall goal of phase III (MARVEL Digital Infrastructure) and, in particular, will make sure that the activities of MARVEL continue beyond 2026 within the established laboratories at PSI and Empa.

[3] https://github.com/nanotech-empa/aiida-nanotech-empa/

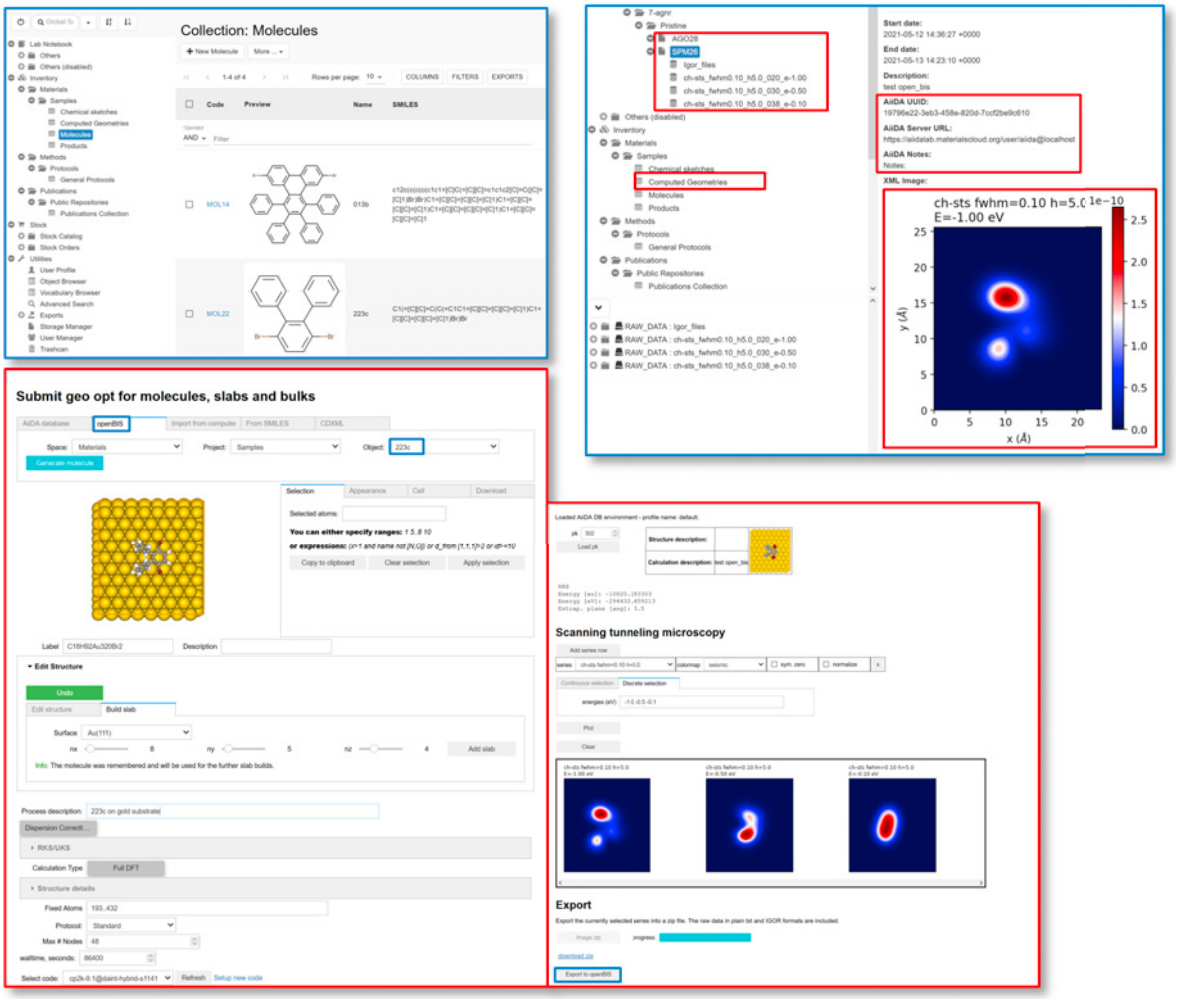


Figure 4: *Screenshot of a preliminary mock-up implementation of the integration of an ELN-LIMS with AiiDAlab to provide a unique open research data (ORD) solution to treat at the same level computational and experimental data. The inventories of experimental apparatus, chemical substances, and experimental procedures (openBIS, top two panels) allow on the one hand to record details of an experiment. On the other hand, the substances' inventory is accessible to the AiiDAlab platform (bottom panels) where simulations for a specific substance on a given substrate can be executed. The results of the simulations can be explored on the AiiDAlab platform but also pushed back to the openBIS platform (highlighted in red in the top right panel), where they become an integral part of the tracking of the experimental steps.*

3 Collaborative and interdisciplinary components

The efforts on XPS and XAS are taking place also in close collaboration with the H2020 project BIG-MAP (part of Battery 2030+), and the group of Dr. Deborah Prezzi at the University of Modena. The efforts in vibrational spectroscopies involve also the University of Bremen. There is currently a working group between the Neutron and Muon division of PSI and the Laboratory of Materials Simulations to collaborate on model Hamiltonianas and muon rest sites. Empa and PSI work together at the development of AiiDAlab, and they have recently secured an open research data (ORD) grant from the ETH domain to integrate AiiDA and electronic lab notebooks.

MARVEL publications

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

- [1] N. Colonna, N. L. Nguyen, A. Ferretti, and N. Marzari, *Koopmans-Compliant Functionals and Potentials and Their Application to the GW100 Test Set*, Journal of Chemical Theory and Computation **15**, 1905 (2019).
- [2] R. D. Gennaro, N. Colonna, E. Linscott, and N. Marzari, *Bloch's theorem in orbital-density-dependent functionals: Band structures from Koopmans spectral functionals*, Physical Review B **106**, 035106 (2022).
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- [4] I. Timrov, F. Aquilante, M. Cococcioni, and N. Marzari, *Accurate Electronic Properties and Intercalation Voltages of Olivine-Type Li-Ion Cathode*

Materials from Extended Hubbard Functionals, PRX Energy **1**, 033003 (2022).

- [5] I. Timrov, N. Marzari, and M. Cococcioni, *HP – A code for the calculation of Hubbard parameters using density-functional perturbation theory*, Computer Physics Communications **279**, 108455 (2022).
- [6] I. Timrov, N. Marzari, and M. Cococcioni, *Hubbard parameters from density-functional perturbation theory*, Physical Review B **98**, 085127 (2018).
- [7] L. Bastonero and N. Marzari, *Calculations of Raman spectra using AiiDA, in preparation* (2023).
- [8] K. Eimre, J. I. Urgel, H. Hayashi, M. Di Giovannantonio, P. Ruffieux, S. Sato, S. Otomo, Y. S. Chan, N. Aratani, D. Passerone, O. Gröning, H. Yamada, R. Fasel, and C. A. Pignedoli, *On-surface synthesis and characterization of nitrogen-substituted undecacenes*, Nature Communications **13**, 511 (2022).
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[11] A. H. Larsen, J. J. Mortensen, J. Blomqvist, I. E. Castelli, R. Christensen, M. Dulak, J. Friis, M. N. Groves, B. Hammer, C. Hargus, E. D. Hermes, P. C. Jennings, P. B. Jensen, J. Kermode, J. R. Kitchin, E. L. Kolsbjerg, J. Kubal, K. Kaasbjerg, S. Lysgaard, J. B. Maronsson, T. Maxson, T. Olsen, L. Pastewka, A. Peterson, C. Rostgaard, J. Schiøtz, O. Schütt, M. Strange, K. S. Thygesen, T. Vegge, L. Vilhelmsen, M. Walter, Z. Zeng, and K. W. Jacobsen, *The atomic simulation environment - a Python library for working with atoms*, Journal of Physics: Condensed Matter **29**, 273002 (2017).

[12] P. Umari and A. Pasquarello, *Infrared and Raman spectra of disordered materials from first principles*, Diamond and Related Materials **14**, 1255 (2005), sMAC '04 Conference Proceeding S.I.

List of year 9 publications related to Pillar 4

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).

⬢○ N. Biniskos, F. J. dos Santos, K. Schmalzl, S. Raymond, M. dos Santos Dias, J. Persson, N. Marzari, S. Blügel, S. Lounis, and T. Brückel
Complex magnetic structure and spin waves of the noncollinear antiferromagnet Mn_5Si_3
Physical Review B **105**, 104404 (2022).
Group(s): Marzari / Project(s): OSP, P4
Related datasets: doi.org/10.24435/materialscloud:85-ys

⬢○ M. Kotiuga, S. Halilov, B. Kozinsky, M. Fornari, N. Marzari, and G. Pizzi
Microscopic picture of paraelectric perovskites from structural prototypes
Physical Review Research **4**, L012042 (2022).
Group(s): Marzari, Pizzi / Project(s): P3,P4,OSP
Related datasets: doi.org/10.24435/materialscloud:jc-ky

⬢○ 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).
Group(s): Ceriotti, Marzari, Pizzi / Project(s): P2, P3, P4
Related datasets: doi.org/10.24435/materialscloud:9g-k6

⬢○ D. Campi, N. Mounet, M. Gibertini, G. Pizzi, and N. Marzari
Novel materials in the Materials Cloud 2D database
arXiv:2210.11301 (2022).
Group(s): Marzari, Pizzi / Project(s): P3, P4, DD3
Related datasets: doi.org/10.24435/materialscloud:36-nd

⬢○ 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
arXiv:2211.16925 (2022).
Group(s): Marzari / Project(s): P4
Related datasets: doi.org/10.24435/materialscloud:xq-5d

⬢○ F. J. dos Santos and N. Marzari
Fermi energy determination for advanced smearing techniques
arXiv:2212.07988 (2022).
Group(s): Marzari / Project(s): OSP, P4
Related datasets: not applicable

Advanced Simulation Methods

Advanced Simulation Methods: From Materials to Devices

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

Partner: Michael Schüler (UniFR)

1 Progress of the different efforts

The main achievements of the ETH Zurich and Empa groups have been the realistic simulation of electron transport through WS_2 monolayers and the development of an efficient projected-GW method. The PSI/UniFR groups have demonstrated the potential of circular-dichroism RIXS as a tool for measuring orbital angular momentum textures.

1.1 *Ab initio* GW+DMFT

A new PhD student, Ruslan Mushkaev, has been hired at UniFR for the GW+DMFT effort, whose goal is to develop a user-friendly GW+DMFT *ab initio* simulation framework. With the help of former MAFVEL postdoc Francesco Petocchi and PhD student Viktor Christiansson, Ruslan Mushkaev has familiarized himself with the existing GW+DMFT code and with the *ab initio* input generation based on FLEUR and SPEX. As a warm-up project, the previous *ab initio* calculations for $SrVO_3$ [1] have been extended from a 3-band (t_{2g}) model to a 12-band model, which includes e_g, t_{2g} and oxygen states. The comparison between the t_{2g} spectral functions for the 3-band and 12-band models is shown in Fig. 1. Both results reproduce the previously identified plasmon satellite at $\omega \approx 2$ eV, which also leaves a clear trace in the frequency-dependent effective interaction (not shown).
Between June and December 2022, the project has rested, since Ruslan Mushkaev had to do the military service.

1.2 Resonant inelastic X-ray scattering (RIXS)

In a collaboration between PSI and UniFR, Michael Schüler, Thorsten Schmitt and Philipp Werner explored to what extend circular dichroism (CD) in RIXS can be used to extract information on the orbital angular momentum texture in complex materials [2]. Based on accurate modeling with first-principles treatment of the light-matter interaction, dichroic RIXS spectra were computed for the prototypical transition metal dichalcogenide $MoSe_2$ and for the two-dimensional topological insulator $1T'$-MoS_2. Guided by an intuitive picture for the optical selection rules, it was shown how the momentum-dependent orbital angular momentum manifests itself in the dichroic RIXS signal if the measurement setup provides control over the momentum transfer. This is demonstrated in Fig. 2 for the case of $MoSe_2$. Momentum transfer along the x direction has different effects on the K and K′ valleys (Fig. 2b) which results in a characteristic signal in CD RIXS as shown in Fig. 2a. On the other hand, for momentum transfer along the y direction, the contributions from the K and K′ valleys cancel (Fig. 2c), which results in vanishing circular dichroism.
These calculations, which were performed for typical experimental geometries and parameters, demonstrate the possibility of observing the predicted circular dichroism in future ex-

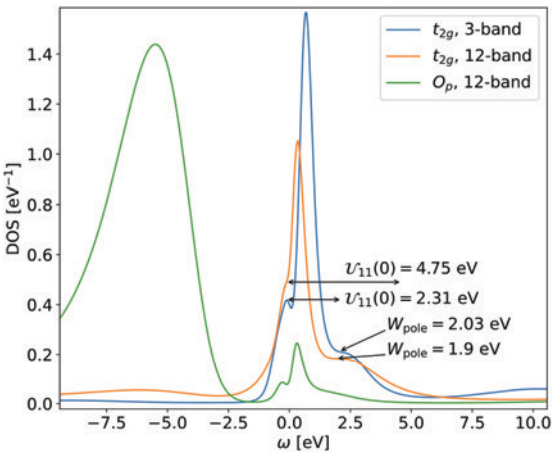

Figure 1: *t_{2g} spectral functions for $SrVO_3$ obtained with ab initio GW+DMFT using a 3-band model (blue) and a 12-band model (orange). The green line shows the spectral function for the oxygen states in the 12-band model.*

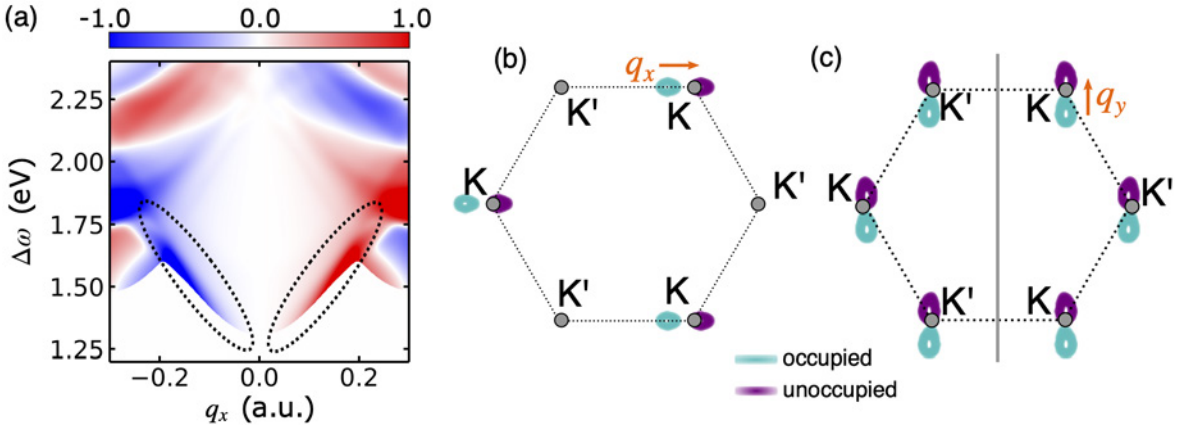

Figure 2: *Circular dichroism in RIXS from $MoSe_2$. (a) Normalized circular dichroism of the RIXS cross section $(I_{LCD} - I_{RCD})/(I_{LCD} - I_{RCD})$. Here, I_{LCD} and I_{LCD} denote the RIXS intensity for left-circularly polarized and right-circularly polarized light, respectively. (b) Sketch of the d-d excitations permitted by energy and momentum conservation at fixed momentum transfer $q_x = 0.164$ a. u. and energy loss $\Delta\omega = 1.73$ eV. (c) Analogous sketch for the momentum transfer in the y direction.*

periments.

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

The Luisier group was completed at the beginning of MARVEL phase III by two new PhD students, Nicolas Vetsch and Mauro Dossena, who were added to Guido Gandus and Youseung Lee. Both Guido Gandus and Youseung Lee were already involved in phase II. Nicolas Vetsch's thesis will focus on the development of quantum transport methods to investigate light-matter interactions in 2D materials, in particular their van der Waals heterojunctions, while Mauro Dossena will work on the impact of defects at semiconductor-oxide interfaces on the transport properties of next-generation transistors with a WS_2 monolayer channel, one of the most promising transition metal dichalcogenides.

Results from MARVEL year 9 at ETH Zurich are highlighted in Fig. 3. First, Fig. 3a shows the energetically-resolved transmission function of electrons injected into WS_2 monolayers onto which an Al_2O_3 insulator was deposited. This data was computed with the OMEN quantum transport solver where the required Hamiltonian and overlap matrices were created with the CP2K DFT package. All atomic structures were generated at imec, in Belgium, in the groups of Geoffrey Pourtois. The fact that the transmission functions do not exhibit a step-like behavior, as in the ballistic case, and decrease when the channel length increases indicates that transport is diffusive and that the carrier mobility is limited by the defects at the semiconductor-oxide interface. As next step, mobility values will be extracted for different passivation schemes and various oxides (Al_2O_3, HfO_2, SiO_2, and novel 2D insulators). The final goal will be to identify oxide layers that preserve the high electron and hole intrinsic mobility of WS_2.

Fig. 3b represents a novel scheme called projected-GW (p-GW) that was developed by Guido Gandus to apply GW corrections to DFT inputs within the Non-equilibrium Green's Function (NEGF) framework. It was specifically designed to accurately model the energy levels of quasi-particle correlated defects in 2D materials. One key aspect of the method is that it avoids the interaction of defects with their periodic images. This is achieved by using open boundary conditions around defect locations, which removes their periodic replica and possible interactions with them. By comparing two different WS_2 defect states (sulfur vacancy and adatom) to available theoretical and experimental data, it could be confirmed that the proposed GW correction to the DFT defect levels delivers accurate results [3]. The machinery is now in place to simulate the "current vs voltage" characteristics of transistors with a 2D channel and to explore how defects impact other 2D materials, besides WS_2.

In Fig. 3c and d, the effects of optical illumination on a $MoSe_2$-WSe_2 van der Waals heterostrutures (vdWH) can be observed. Electron-photon interactions were added to the OMEN quantum transport solver through non-diagonal scattering self-energies [4]. All inputs (Hamiltonian matrices and impulse operators) are calculated at the *ab initio* level using maximally localized Wannier functions (MLWFs) in the present case. Current conserva-

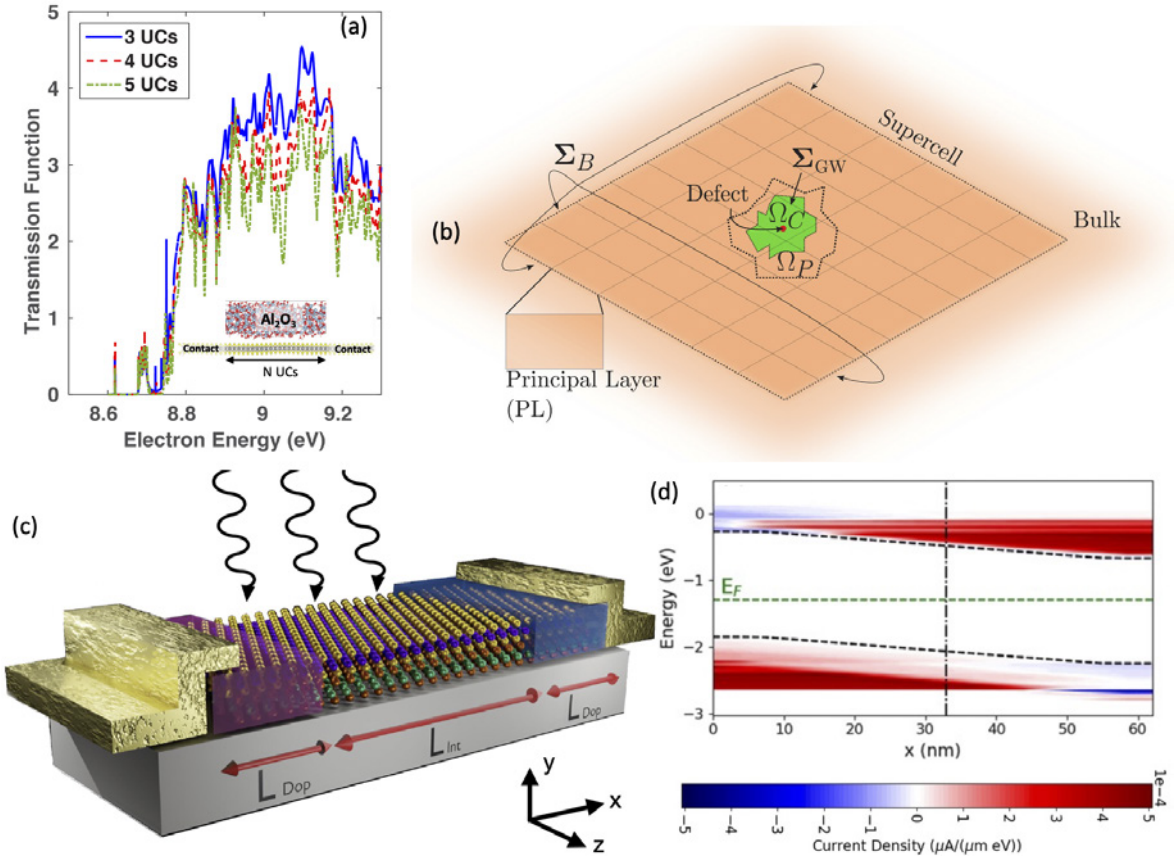

Figure 3: *Overview of the work performed at ETH Zurich. (a) Energetically-resolved transmission function through WS_2-Al_2O_3 transistors as a function of their channel length (2, 3, and 4 unit cells). Disorder at the semiconductor-oxide interfaces alters electron transport. (b) Developed projected-GW method in collaboration with Empa to only locally account for GW bandgap corrections and thus reduce the computation burden. This approach was implemented in a quantum transport solver to study the influence on defects on the transport properties of MoS_2. (c) Schematic view of a $MoSe_2$-WSe_2 van der Waals heterojunction under light illumination. (d) Photo-induced electrical current in the P-I-N structure shown in (c). Electron-hole pairs are generated through photon absorption and then accelerated by the electric field towards the electrodes.*

tion is ensured, which allows to identify the locations where electrons and holes are generated and where the corresponding electrical currents flow. This model was used to reveal under which conditions inter-layer electron-hole pairs can be created: this process involves states, typically from the valence band, that are delocalized over the two monolayers constituting the vdWH.

In 2022, the Luisier group also conducted research on the thermal transport properties of MoS_2-hBN transistors, shedding light on the role played by the phonons coming from the hBN layer [5], and on the realization of double quantum dot systems in bilayer graphene [6].

1.4 Correlations in realistic materials

During the year 2022, the integration of the methods developed by Guido Gandus and aimed at blending DFT, GW, DMFT and NEGF approaches has proceeded as planned. In addition to the already cited p-GW scheme, an important milestone has been the inclusion of the local orbitals scheme developed with Angelo Valli in 2020-2021 in the popular suite GPAW. Concerning the transport simulations in realistic materials, two publications (one submitted to arXiv [7], the other to be submitted) have been prepared concerning side and flat contacting of 9-armchair graphene nanoribbons to metallic leads, and the connected electronic transport properties. In the collaboration with the Perrin/Calame group at Empa, DFT and NEGF have been employed to show a favorable contact resistance and transmission function, particularly in the case of side contacts of the ribbons protected by a h-BN layer. Starting in 2023 the Passerone group at Empa will be enriched by a theoretical postdoc co-financed by this NCCR and Empa director's board. This scientist will continue both the methodological developments by Guido Gandus as well as the applications to modeling of nanoelectronics

and nanodevices.

2 Contribution to overall goals and initial proposal

Progress at UniFR has been slow, because the hired PhD student spent the second half of 2022 doing his military service. Apart from this, the GW+DMFT effort is on track to meet the goals for MARVEL phase III.
The work at ETH Zurich is progressing according to the proposal for MARVEL's phase III: advanced, *ab initio* models are developed to simulate electrical, optical, and thermal transport in 2D materials and other nanoscale devices. Methods to automatically create the necessary input quantities are implemented, with a focus on light-matter interactions during year 9.

3 Collaborative and interdisciplinary components

PSI and UniFR are collaborating on RIXS related problems and other projects related to light-matter interactions. Apart from the CD RIXS project mentioned in this report, there is an ongoing collaboration involving PhD student Markus Lysne on measuring the quantum metric of materials in cavity setups.
ETH Zurich and Empa are intensively collaborating with each other on the *ab initio* exploration of different metals to contact ultra-narrow graphene nanoribbons. Moreover, they developed together the aforementioned p-GW method. Besides Empa, ETH Zurich studied the impact of defects on the optical absorption of bilayer $PtSe_2$ with the group of Prof. Andras Kis at EPFL. They also collaborated with Dr. Geoffrey Pourtois at imec (Belgium) on the creation of atomic interfaces between 2D semiconductors and oxides.

MARVEL publications

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

- [1] L. Boehnke, F. Nilsson, F. Aryasetiawan, and P. Werner, *When strong correlations become weak: Consistent merging of GW and DMFT*, Physical Review B **94**, 201106 (2016).
- [2] M. Schüler, T. Schmitt, and P. Werner, *Probing magnetic orbitals and Berry curvature with circular dichroism in resonant inelastic X-ray scattering*, npj Quantum Materials **8**, 6 (2023).
- [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] J. Cao, S. Fiore, C. Klinkert, N. Vetsch, and M. Luisier, *Light-matter interactions in van der Waals photodiodes from first principles*, Physical Review B **106**, 035306 (2022).
- [5] S. Fiore, C. Klinkert, F. Ducry, J. Backman, and M. Luisier, *Influence of the hBN Dielectric Layers on the Quantum Transport Properties of MoS_2 Transistors*, Materials **15**, 1062 (2022).
- [6] J. Cao, G. Gandus, T. Agarwal, M. Luisier, and Y. Lee, *Dynamics of van der Waals charge qubit in two-dimensional bilayer materials: Ab initio quantum transport and qubit measurement*, Physical Review Research **4**, 043073 (2022).
- [7] G. Gandus, D. Passerone, R. Stadler, M. Luisier, and A. Valli, *Strongly correlated physics in organic open-shell quantum systems*, arXiv:2301.00282 (2023).

List of year 9 publications related to Advanced Simulation Methods 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).

⬢○ J. Chen, F. Petocchi, and P. Werner
Causal versus local GW+ EDMFT scheme and application to the triangular-lattice extended Hubbard model
Physical Review B **105**, 085102 (2022).
Group(s): Werner / Project(s): ASM
Related datasets: not applicable

○ V. Christiansson, F. Petocchi, and P. Werner
Superconductivity in black phosphorus and the role of dynamical screening
Physical Review B **105**, 174513 (2022).
Group(s): Werner / Project(s): ASM
Related datasets: not applicable

⬢○ S. Fiore, C. Klinkert, F. Ducry, J. Backman, and M. Luisier
Influence of the hBN Dielectric Layers on the Quantum Transport Properties of MoS_2 Transistors
Materials **15**, 1062 (2022).
Group(s): Luisier / Project(s): ASM
Related datasets: doi.org/10.24435/materialscloud:7f-5t

⬢○ C. Nicholson, F. Petocchi, B. Salzman, C. Witteveen, M. Rumo, G. Kremer, F. von Rohr, P. Werner, and C. Monney
Modified interlayer stacking and insulator to correlated-metal transition driven by uniaxial strain in 1T-TaS_2
arXiv:2204.05598 (2022).
Group(s): Werner / Project(s): ASM
Related datasets: not applicable

⬢○ F. Petocchi, C. Nicholson, B. Salzmann, D. Pasquier, O. Yazyev, C. Monney, and P. Werner
Mott versus Hybridization Gap in the Low-Temperature Phase of 1T-TaS_2
Physical Review Letters **129**, 016402 (2022).
Group(s): Werner, Yazyev / Project(s): ASM, DD5, DD6
Related datasets: doi.org/10.24435/materialscloud:v6-nk

⬢○ J. Cao, S. Fiore, C. Klinkert, N. Vetsch, and M. Luisier
Light-matter interactions in van der Waals photodiodes from first principles
Physical Review B **106**, 035306 (2022).
Group(s): Luisier / Project(s): ASM
Related datasets: doi.org/10.24435/materialscloud:2z-33

⬢○ J. Cao, G. Gandus, T. Agarwal, M. Luisier, and Y. Lee
Dynamics of van der Waals charge qubit in two-dimensional bilayer materials: Ab initio quantum transport and qubit measurement
Physical Review Research **4**, 043073 (2022).
Group(s): Luisier / Project(s): ASM
Related datasets: doi.org/10.24435/materialscloud:nh-nk

⬢○ G. Gandus, D. Passerone, R. Stadler, M. Luisier, and A. Valli
Strongly correlated physics in organic open-shell quantum systems
arXiv:2301.00282 (2023).
Group(s): Luisier, Passerone / Project(s): ASM
Related datasets: not applicable

⬢○ 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).
Group(s): Luisier, Passerone / Project(s): ASM
Related datasets: doi.org/10.24435/materialscloud:h4-c0

⬢ M. Schüler, T. Schmitt, and P. Werner
Probing magnetic orbitals and Berry curvature with circular dichroism in resonant inelastic X-ray scattering
npj Quantum Materials **8**, 6 (2023).
Group(s): Schüler, Werner / Project(s): ASM
Related datasets: doi.org/10.24435/materialscloud:ck-7m

Quantum Simulations

Leveraging Quantum Computers and Algorithms for Materials Discovery

Project leader: Giuseppe Carleo (EPFL)

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

1 Progress of the different efforts

1.1 Overview

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 wave functions 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 wave functions for material classification and property prediction.

The project's first months have been devoted to introducing core techniques that will be instrumental in developing the points highlighted above. As also presented in the proposal, the key methodological aspect we want to explore is the ability to leverage small quantum computers to study electronic systems potentially much larger than the available number of physical qubits. In this first phase, we have focused on quantum embedding techniques, which are instrumental in achieving this goal.
In particular, the effort around quantum embeddings has been twofold. On the one hand, we started the development of integration with classical methods such as neural quantum states [4] or density matrix embedding theory (DMET) [5, 6] to extend the reach of currently available quantum hardware. On the other hand, we have focused on density functional theory (DFT) embeddings, given their importance in connecting to classical electronic structure codes. This scheme allows studying molecular systems and localized defect systems. In particular, the coupling of the quantum driver Qiskit with the high-performance Hartree-Fock (HF) and DFT software package CP2K is used. A complete refactoring of Qiskit now allows for more flexible interfaces to classical codes. Currently, CP2K is adapted to the use of this new Qiskit API for the development of a computationally efficient quantum computing/classical computing (QC/CC) active space embedding scheme that can be applied in the study of metalorganic complexes, which are difficult to simulate with pure DFT approaches.
Finally, in an effort to move towards studying dynamical properties with the methods developed while keeping in check the size of the quantum hardware, we have started exploring the possibility of combining quantum embeddings with variational dynamics. In this context, we have applied the variational quantum eigensolver (VQE), an already successful quantum algorithm, to studying dynamics [1].

1.2 Description of the project progress

As stated in the research plan, the main focus of year 9 has been on assessing the quantum hardware requirements and its capabilities to estimate static and dynamic properties of electronic structures on quantum hardware in the near term.

a) *Dynamics on a quantum device as a ground state problem* The variational quantum eigensolver (VQE) [7] is one of the most successfully applied quantum algorithms due to its natural robustness to certain types of errors that occcur on current hardware. On the other hand, quantum dynamics can be efficiently simulated on

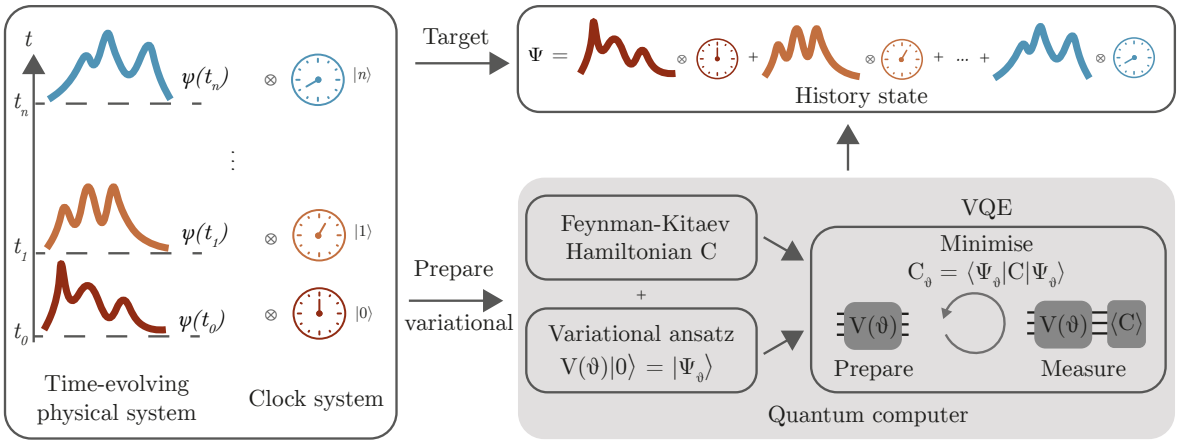

Figure 1: *Coupling the physical system to an auxiliary clock system we can encode an entire time evolution into a time-independent state. We prepare a variational approximation of the history state using the VQE algorithm.*

quantum hardware, but the current simulations are limited to short times in the absence of quantum error correction schemes.
In this project, we mitigate this problem by applying VQE to the study of the dynamics of quantum systems. This result is obtained by encoding time as a quantum degree of freedom using an auxiliary quantum system. Given a time-dependent system, it is possible to construct a Hamiltonian for the joint physical-clock system whose ground state encodes the whole evolution of the original system. Such a construction, originally proposed by Feynman and Kitaev, is effectively recasting the problem of quantum dynamics into a ground-state problem.
We show how to efficiently map the Feynman-Kitaev Hamiltonian to quantum hardware and assess the computational cost of measuring it, proposing an efficient scheme that runs in polynomial time. Finally, we test the method on the transverse Ising model, measuring dynamical phase transitions. The findings of this project have been published in *Physical Review Research* [1], a sketch of the algorithm can be found in Fig. 1.

b) *Hybrid quantum-classical variational ansatz* Simulation of quantum chemical and physical systems is one of the most envisioned applications of quantum computers. However, given that quantum resources are still limited in size and coherence times, these demonstrations have focused on small molecular and spin systems. In particular, treating entire systems of technological relevance is unlikely to be a realistic near-term proposition. To scale up to more complex applications, it is highly desirable to introduce novel approaches that combine quantum algorithms with classical computational methods and keep quantum resources under control.
In this project we introduce a completely variational ansatz combining a neural network and a parameterized quantum circuit in order to determine the ground state of quantum systems. To this aim, the machine learning models obtained with NetKet [8] are interfaced with quantum circuits created in Pennylane [9]. In the initial phase, we estimated the amount of classical and quantum resources to evaluate physical quantities and optimize the variational parameters. Then, to assess the performance of the method, we performed some preliminary calculations on spin systems. Further steps will consist of the application of the method to correlated systems such as molecular electronic structures. Stefano Barison, in the Carleo group, is the PhD student who is working on this project.

c) *Time-dependent quantum-classical hybrid embedding* Quantum computation is expected to enable us to solve strongly-correlated systems with high accuracy using resources that scale linearly in the system size. However, near-term hardware drastically limits the number of qubits available and is prone to noise. In the foreseeable future, we will thus not be able to solve a big system on a single quantum processing unit (QPU). In this project, we aim to mediate this problem by splitting the big system into clusters, where a single cluster is small enough for the solution to be implementable on a QPU but still too expensive to solve classically. We can then treat one cluster at the time as the fragment of the system that we solve on a QPU whereas the remaining clusters are treated as a bath using a classical low-level method. Different such embedding schemes have been proposed classically [10]. Especially density matrix embedding theory

(DMET) [5, 6] is a promising candidate for a hybrid embedding scheme.

Gian Gentinetta has recently started his PhD with Giuseppe Carleo and is investigating how hybrid quantum-classical embeddings can be realized and, in a further step, analyzes how we can use embeddings to solve time-dependent problems. For the latter, we plan to make use of the time-dependent variational principle [11] to constrain the solution of the time-dependent Schrödinger equation to the embedding space. Another way of seeing these embedding schemes is the generalization of the so-called entanglement forging [12, 13], where we classically forge entanglement between several QPUs.

d) *Periodic quantum-classical hybrid embedding* A number of technologically relevant applications are based on localized features in solid state materials, e.g., point defects and vacancies. Quantum embedding methodologies provide an ideal approach to couple a high-level description of these *impurities* with a low-level representation of the environment. Importantly, owing to the (typically) small size of the impurity, we can leverage the advantage of near-term QPUs to obtain the high-level description, while using classical algorithms, e.g. density functional theory, to compute the effects of the bath.

Stefano Battaglia has recently started a postdoc position with Jürg Hutter and is currently interfacing CP2K to IBM's Qiskit Nature library in collaboration with Max Rossmannek (PhD student with Ivano Tavernelli). This development extends the use of the range-separated WFT-in-DFT quantum embedding approach [14, 15] from molecules to condensed matter systems, whereby the environment can be treated with periodic boundary conditions. In the future, Battaglia will investigate the possibility to use this approach to study locally excited states on the impurity, as found in, e.g., color centers.

Furthermore, the implemented interface enables CP2K to communicate to other classical codes as well, opening up the possibility to perform periodic embedding calculations using other impurity solvers, such as quantum Monte Carlo and the density matrix renormalization group.

e) *Integrating quantum computing into classical quantum chemistry codes* In the last six months, Rossmannek extensively worked on refactoring IBM's open-source software package, Qiskit Nature[1], which enables the simulation of natural science problems on quantum computers. As of version 0.5, Qiskit Nature supports a plugin-like integration into existing classical-computing quantum chemistry codes to be used as a quantum-powered active space or impurity solver. While Python-based integrations already exist for PySCF[2], Psi4[3] and Gaussian[4], the refactoring will allow tighter integrations into the classical codes themselves. This enables more complex workflows for hybrid algorithms and can already be seen in action with the Qiskit Nature PySCF plugin[5].

2 Contribution to overall goals and initial proposal

The research contributions presented above align with our original proposal, and we are moving towards achieving the main goals stated. The quantum embedding techniques we are developing are especially important for the project's future and will constitute the core of our research activities for at least another year. Concerning other aspects presented in the original proposal, there has been progress around some directions with lower priority.

For example, to mitigate quantum computing error induced by qubit decoherence times and qubit operation infidelities, we have investigated the implementation of quantum correlation functions, such as the one-body Greens function, using both real-time and frequency space representations. Both implementations confirm this novel approach's validity and stability for studying many-body properties in periodic systems. Two articles on this topic were published in the course of 2022 [2, 3]. An example of the Green's function computed for the 2-side Hubbard model is given in Fig. 2.

Finally, we also developed ways to mitigate the statistical errors arising in the measurement process of a quantum state on a quantum computer. The approach is based on informationally complete positive operator valued measures (IC-POVM), which can save one to two orders of magnitude in the number of shots needed to achieve the desired accuracy [16].

Concerning the project on quantum machine learning for material classification, we are still in the phase of recruting the assigned PhD student. A progress report on this topic will be

[1] https://github.com/Qiskit/qiskit-nature/tree/stable/0.5/
[2] https://pyscf.org/
[3] https://psicode.org/
[4] https://gaussian.com/gaussian16/
[5] https://github.com/qiskit-community/qiskit-nature-pyscf/

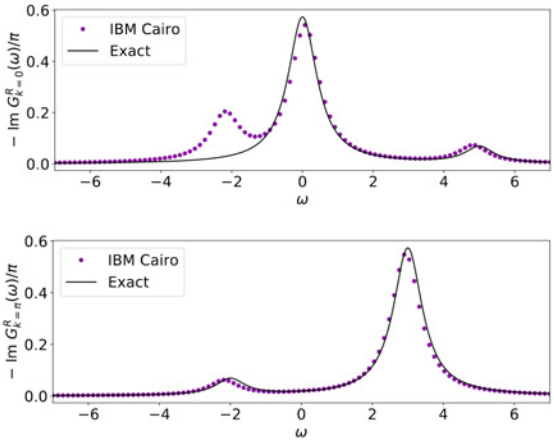

Figure 2: *Imaginary part of the Green's functions for the 2 side Hubbard model computed on the IBM quantum device ibm_cairo (red dots) and from exact simulations (black lines) for $k = 0$ (upper panel) and $k = \pi$ (lower panel).*

presented in the next report.

3 Collaborative and interdisciplinary components

In this first phase, there have been direct collaborations within the Quantum Simulations project, especially related to integrating software. Specifically, Rossmannek and Battaglia are working to integrate Qiskit Nature and CP2K. This will enable the extensions of Qiskit functionalities to the quantum chemistry of periodic systems, liquids, materials, and crystals, paving the way for simulations in material science. Of particular relevance for the quantum computing community is the possibility to leverage the complex functionalities of CP2K, such as molecular dynamics, enhanced sampling techniques, and excited states properties for periodic systems, which the combined Gaussian and plane waves basis sets enable. This basic development way lay the foundation for the next steps in our research project, namely the study of defects in periodic systems using a hybrid quantum computing/ quantum computing approach.

MARVEL publications

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

- [1] S. Barison, F. Vicentini, I. Cirac, and G. Carleo, *Variational dynamics as a ground-state problem on a quantum computer*, Physical Review Research **4**, 043161 (2022).
- [2] F. Libbi, J. Rizzo, F. Tacchino, N. Marzari, and I. Tavernelli, *Effective calculation of the Green's function in the time domain on near-term quantum processors*, Physical Review Research **4**, 043038 (2022).
- [3] J. Rizzo, F. Libbi, F. Tacchino, P. J. Ollitrault, N. Marzari, and I. Tavernelli, *One-particle Green's functions from the quantum equation of motion algorithm*, Physical Review Research **4**, 043011 (2022).

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[6] G. Knizia and G. K.-L. Chan, *Density Matrix Embedding: A Strong-Coupling Quantum Embedding Theory*, Journal of Chemical Theory and Computation **9**, 1428 (2013).

[7] A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien, *A variational eigenvalue solver on a photonic quantum processor*, Nature Communications **5**, 4213 (2014).

[8] F. Vicentini, D. Hofmann, A. Szabo, D. Wu, C. Roth, C. Giuliani, G. Pescia, J. Nys, V. Vargas-Calderon, N. Astrakhantsev, and G. Carleo, *NetKet 3: Machine Learning Toolbox for Many Body Quantum Systems*, SciPost Physics Codebases **7** (2022), doi:10.21468/SciPostPhysCodeb.7.

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[10] Q. Sun and G. K.-L. Chan, *Quantum Embedding Theories*, Accounts of Chemical Research **49**, 2705 (2016).

[11] A. D. McLachlan, *A variational solution of the time-dependent Schrodinger equation*, Molecular Physics **8**, 39 (1964).

[12] A. Eddins, M. Motta, T. P. Gujarati, S. Bravyi, A. Mezzacapo, C. Hadfield, and S. Sheldon, *Doubling the Size of Quantum Simulators by Entanglement Forging*, PRX Quantum **3**, 010309 (2022).

[13] P. Huembeli, G. Carleo, and A. Mezzacapo, *Entanglement Forging with generative neural network models*, arXiv:2205.00933 (2022).

[14] E. Fromager, J. Toulouse, and H. J. A. Jensen, *On the universality of the long-/short-range separation in multi-configurational density-functional theory*, The Journal of Chemical Physics **126**, 74111 (2007).

[15] 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).

[16] G. García-Pérez, M. A. Rossi, B. Sokolov, F. Tacchino, P. K. Barkoutsos, G. Mazzola, I. Tavernelli, and S. Maniscalco, *Learning to Measure: Adaptive Informationally Complete Generalized Measurements for Quantum Algorithms*, PRX Quantum **2**, 040342 (2021).

List of year 9 publications related to the Quantum Simulations 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).

⬢○ S. Barison, F. Vicentini, I. Cirac, and G. Carleo
Variational dynamics as a ground-state problem on a quantum computer
Physical Review Research **4**, 043161 (2022).
Group(s): Carleo / Project(s): QS
Related datasets: doi.org/10.24435/materialscloud:xf-wj

⬢○ F. Libbi, J. Rizzo, F. Tacchino, N. Marzari, and I. Tavernelli
Effective calculation of the Green's function in the time domain on near-term quantum processors
Physical Review Research **4**, 043038 (2022).
Group(s): Marzari, Tavernelli / Project(s): QS
Related datasets: not applicable

⬢○ J. Rizzo, F. Libbi, F. Tacchino, P. J. Ollitrault, N. Marzari, and I. Tavernelli
One-particle Green's functions from the quantum equation of motion algorithm
Physical Review Research **4**, 043011 (2022).
Group(s): Marzari, Tavernelli / Project(s): QS
Related datasets: not applicable

4.3 List of new projects

As mentioned in the full proposal for phase III, UniFR and PSI were planning to jointly hire 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. This was done, in the person of Michael Schüler, joining UniFR and PSI in September 2022 and MARVEL as group leader in the Advanced Simulation Methods project. He brings spectroscopy experience to merge theory and experiment in MARVEL's phase III.
As he says in his interview by Carey Sargent, "the nice thing about MARVEL is the synergies that we can generate and benefit from. It is a very lively community. It's really wonderful and I think that with this new Laboratory for Materials Simulations lead by Nicola Marzari at PSI, it will be one of the best spots to exploit these synergies."

5 Structure-related aspects

5.1 Education & Training

5.1.1 PhD students and postdocs

In the MARVEL community

Junior seminars

MARVEL junior seminars are a monthly activity which was initially held on campus at EPFL, and were then moved to a virtual format during the pandemic. They aim to intensify interactions between MARVEL junior scientists from different research groups. In 2022, junior seminars were held until March, and April featured several junior researcher presentations at the phase II closing event. They were interrupted by the buildup to the Psi-k 2022 conference, but will now be launched again in a hybrid format, following the formation of a renewed MARVEL community for phase III. More details are given in section 5.4 on Communication & Outreach.

Summer schools

A group of MARVEL PhD students organized a summer school entitled "Advanced Electronic Structure Methods in Condensed Matter Physics" in 2019, and obtained ETH Board funding for their school. As they wished to organize their effort somewhat independently of MARVEL and due to significant overlap with MARVEL themes, the NCCR opted to fully promote and support the effort of these students by providing significant sponsorship and by covering the registration costs for MARVEL members instead of organizing a competing junior retreat. A similar arrangement was planned for 2020, with the NCCR supporting a summer school organized by MARVEL junior researchers, but it could not take place due to the pandemic, and was postponed first to 2021, and then to 2022.

The event was remodeled as a workshop entitled "First-principles modelling of defects in solids"[1] and took place June 13–15, 2022 at ETH Zurich. The school attracted 84 participants from 32 institutions in 16 countries. Each day of the three-day conference was assigned a thematic track, respectively: point defects from density functional theory (DFT), defects beyond DFT: machine learning and emergent approaches, and defects in low-dimensional systems and electronic devices.

Talks by well-known names in the field (Van de Walle, Valenti and Yazyev), as well as by some researchers earlier in their careers, made a big impression on the audience. The poster session was very interactive and one of the important highlights of the conference as it gave students an excellent opportunity to present their own work.

Education platform

a) *OSSCAR* Open Software Services for Classroom and Research (OSSCAR)[2] provides a platform to develop, deploy, access and share material for teaching and learning in the form of web applications. Content relates to specific topics and illustrates them via interactive Jupyter notebooks that include bespoke and interactive visualization tools. Contributions from the community are invited, and are easy to implement for teachers. The project started in 2019 and received funding by the EPFL Open Science Fund.

An online presentation of OSSCAR was given on March 9, 2022, as an opportunity to share this new tool and explore its potential for future collaborations. A number of interactive visualizations were also developed and are available at osscar-quantum-mechanics.materialscloud.io.

[1] sites.google.com/view/defects-in-solids
[2] www.osscar.org

b) *Lhumos* The Learning Hub for Modelling and Simulation (Lhumos) platform is a collaboration between MARVEL, CECAM, and MaX and aims to develop a web portal to collect and disseminate basic and advanced material for continuous training, with particular focus on materials simulations. It will contain videos, lecture notes, links to Git repositories of codes and tutorials, enabling researchers and students to access state-of-the-art training material. It will also provide a hub for institutions or projects that wish to contribute to this community-driven repository. Efforts and progress made on this platform are detailed in the Pillar 3 section of the Research chapter. Lhumos was presented at the Psi-k 2022 conference in August and at the CECAM SCOUT Strategic Workshop in October. Interest was shown from possible future partners, such as the Electronic Structure Library and the Electronic Theoretical Spectroscopy Facility[3], which published a presentation of Lhumos in its newsletter.

CECAM-MARVEL Classics in molecular and materials modeling

MARVEL and CECAM launched in 2019 a series of lectures entitled "Classics in molecular and materials modeling", in which 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.
While the first two events (the first with Jean-Paul Ryckaert and Giovanni Ciccotti, and the second with Michele Parrinello and Roberto Car) were held on site at EPFL and attracted about 40–50 participants, the following two events (David Vanderbilt and Raffaele Resta, then Daan Frenkel and Tony Ladd) 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 fully online version to maximize viewership. We featured Athanassios Panagiotopoulos and Dominic Tildesley in December 2021 (225 unique viewers), followed by Lucia Reining, Rex Godby and Steven Louie in January 2022 (with 370 unique viewers), then Giorgio Parisi and Marc Mézard in November 2022 (with 275 unique viewers), and, most recently, Antoine Georges and Gabriel Kotliar in December 2022 (with 200 unique viewers).

[3] esl.cecam.org/data/etsf_io/

Outside MARVEL

18th ETSF Young Researchers' Meeting

MARVEL supported the 18th ETSF Young Researchers' Meeting, which took place on September 5–9, 2022 in Marseille. The objectives of this meeting were to provide young researchers with the opportunity to share their work and acquaint themselves with state-of-the-art theoretical methods applied both in their own field and in others. Moreover, it offered scientists at the beginning of their careers the chance to network with young colleagues from different institutions, exchange knowledge and ideas and thus integrate further into the scientific community. The meeting included oral sessions dedicated to advanced electronic structure methods, strongly correlated systems, the vibrational properties of materials, the optical properties of materials, as well as multiscale modelling.

Quantum Computing Hardware and Software Summer School

In line with the NCCR's goals on education and training, the Quantum Computing Hardware and Software Summer School (QCHS) was organized at EPFL on June 13–17. Stefano Barison, in the group of Giuseppe Carleo, directed the organizing committee together with Ivan Rojkov (ETH Zurich) and received financial support from the EPFL doctoral school, the Center for Quantum Science and Engineering at EPFL and the ETH Zurich Quantum Center. The summer school gathered more than 50 graduate and master students together with top scientists from all around the globe (Fig. 1)

Figure 1: *Picture of the QCHS 2022 participants.*

to discuss the most recent advances in the field of quantum computation. During the week, participants had the occasion to attend lectures, get involved in workshops with hands-on session on quantum computing libraries, participate in panel sessions with the experts and present their own research during the poster sessions. The aim of the school was twofold: to introduce new, highly motivated students to the field of quantum computation and to connect junior researchers in quantum science and technology to stimulate future collaborative works.
To further extend the reach of the school and give access to those who didn't have the opportunity to attend in person, the whole schedule was also live streamed online using the Twitch platform. The recordings were later uploaded onto the QCHS official YouTube channel. More information can be found on the school's official website.

Other schools

- Berend Smit lectured at the 25th edition of the winter school "Understanding Molecular Simulation" (MolSim -2023), January 9–20, 2023, which attracts 80 PhD students from all over the world each year. The 2023 event will be the last to be based on the 2nd edition of the book *Understanding Molecular Simulation* by Frenkel and Smit; the 2024 school will be based on the completely revised and extended 3rd edition.

- In July, William Curtin taught a day-long, hands-on module on Atomistic Modeling at the Computational Materials Science Summer School run by Texas A&M and funded by the US National Science Foundation. The summer school was attended both in person and virtually by PhD students and post-docs around the world. MARVEL team member Manura Liyanage ran the hands-on sessions using the molecular dynamics code LAMMPS.

- Michele Ceriotti co-organized a summer school on "Theoretical modeling at the nanoscale", July 3–8, at Ringbergschloss, Germany.

- Philipp Werner has given lectures on "nonequilibrium dynamical mean field theory" at the International Summer School on Computational Quantum Materials, June 5–17, in Jouvence (Canada) and, with the help of his PhD students, organized a hands-on tutorial for the NESSi library.

- Philipp Werner has also given lectures on "quantum Monte Carlo impurity solvers" at the autumn school on Dynamical Mean Field Theory of Correlated Electrons, October 4–7, in Jülich (Germany).

Initiatives in sub-Saharan Africa

Machine Learning in Electronic Structure and Molecular Dynamics From May 16 to 20, MARVEL PI Michele Ceriotti and former MARVEL PI Michele Parrinello participated in this culminating workshop in Kigali, Rwanda of the Machine Learning (ML) in Electronic Structure (ES) and Molecular Dynamics (MD) training workshop that began in October 2021. The focus is to train African researchers in ML and its application in ES and MD.

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). In 2022, about €12'000 supported the participation of six researchers from Africa in the Psi-k 2022 conference, covering travel, accommodation, living allowance, and conference fees.

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,

Figure 2: *Fruitful discussions between Steve Ndengué (EAIFR, Kigali, Rwanda) and Garu Gebreyesus (Univ. Accra, Ghana) during the Psi-k 2022 conference.*

namely Marija Stojkovic, under the supervision of Nicola Marzari.
In 2022, Steve Ndengué came to EPFL for a collaborative visit during one month in August (Fig. 2), and also participated in the Psi-k 2022 conference. Ayda Badri, a postdoc there, also visited for 3 weeks in September.

5.1.2 Master students

Advanced modeling online courses

A plan for phase III is to develop structured digital education tools: a library of "advanced modeling courses" including a set of lectures covering different aspects of a modeling technique, complete with lecture notes, self-assessment exercises and (where possible) practical tutorials using actual research software. So far, a first MOOC "Path Integral Methods in Atomistic Simulations" prepared by Michele Ceriotti, has been released and is accessible at tinyurl.com/pimd-mooc. 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.

Courses

The MARVEL website lists the Master- and PhD-level computational courses currently offered at participating institutions and is regularly updated (nccr-marvel.ch/outreach/education-and-training/Courses-Master-level).

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, attracted 22 high school students — 11 women and 11 men — for a full week of lectures, exercises and lab visits built around the theme of scientific programming and atomistic modeling (Fig. 3). Due to COVID-19 restrictions, the 2021 edition could not accept students coming from outside of Switzerland. This was no longer the case in 2022 and, in addition to students from French-, German- and, Italian-speaking parts of Switzerland, we also welcomed students from different European countries (FR, DE, GB, ES, GR, RO) as well as those coming from as far as Morocco and Dubai. Supervised by Michele Ceriotti and EPFL HPC application experts Nicolas Richart and Emmanuel Lanti, a team of six MARVEL volunteer postdocs and PhD students from the groups of Corminboeuf, Ceriotti and Marzari led the students through a basic introduction to Python to applied exercises in cellular automaton, molecular dynamics and machine learning. The week was enhanced by visits to the clusters of SCITAS (the home of high-performance computing at EPFL), the Swiss Plasma Center, and a guided tour of the EPFL Campus. Student evaluations indicated that the week was a success: "I don't want the camp to end. I had such a good time and I really liked Python"; "I will miss this place. Really nice experience"; "The teachers, they are very cheerful and they

Figure 3: *Picture of the MARVEL summer camp* Des atomes aux ordinateurs, à la découverte de la programmation scientifique *participants.*

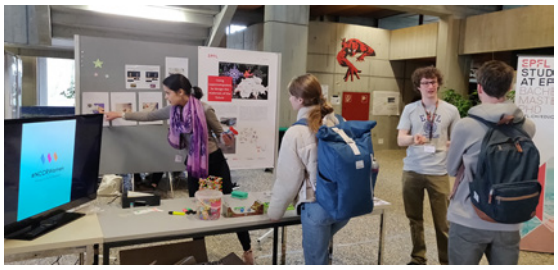

Figure 4: *Thematic day at the at the Gymnasium in Thun on April 7, 2022. On the left, you can see a screen displaying the #NCCRWomen logo.*

always want to help you". A new edition is being planned for the beginning of summer 2023

Thematic day in Thun

The EPFL Education Outreach Department organizes thematic days in high schools that allow students to discover various research domains within their own four walls, with conferences and feature demonstrations. MARVEL participated in the event "Destination Innovation" on April 7 at the *Gymnasium* in Thun (Fig. 4). Building on the #NCCRWomen campaign, in which they both participated, MARVEL PhD students Jigyasa Nigam and Miriam Pougin had a talk centered on the theme of "the journey to becoming a scientist", speaking about what motivated them to do research in the first place as well as explaining their actual scientific work in a way that was intuitive to high school students. They were also present at a stand showcasing MARVEL though hands-on experiments.

Figure 5: *Lab visit during the EPFL information days for high school students on November 25, 2022.*

Other activities

#NCCRWomen in-school — A researcher in my class

As mentioned in section 5.3 on Equal Opportunities, MARVEL is participating in the #NCCRWomen in school, a "researcher in my class" initiative, in which women researchers of MARVEL visit high school classes to present information about who they are, what they do and why they are doing it.

EPFL information days for high school students

Three groups of 8–10 high school students were welcomed in the Marzari group for a lab visit during the EPFL information days for high school students on November 25. Under the supervision of the scientific manager, a female PhD student and a male postdoc presented their research accompanied with hands-on experiments on phonons and practical activities using the interactive visualizations proposed on the OSSCAR platform (Fig. 5).

5.2 Knowledge & Technology Transfer

5.2.1 Knowledge transfer

Software

AiiDA

AiiDA 2.0, 2.1 and 2.2 were released in year 9, and the developments and improvements are presented in the Pillar 3 section of the Research chapter. Beside the code development, one major activity is its dissemination through the scientific community and beyond. In particular,

- the annual AiiDA introductory tutorial was held online on October 4–7 2022, introducing AiiDA to ∼80 researchers across the globe, spanning 34 different nationalities (Fig. 6);
- an additional AiiDA tutorial was held in Antwerp (Belgium) on May 20;
- a 1-week-long summer school on the Wannier90 code (Wannier 2022 summer school) was organized on May 16–20 in ICTP (Trieste, Italy), followed by a 1-week-long developers meeting;
- an AiiDA plug-in developers hackathon was organized in November 2022 at EPFL to help AiiDA plugin developers migrate to AiiDA 2.0 and take advantage of the new code functionalities;
- both AiiDAlab and the AiiDA common workflow interfaces were presented at the 2022 Scientific Python (SciPy) conference in Austin in July, with about 800 participants.

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 news features can be found in the Pillar 3 section. Notably, the Materials Cloud *Archive* is now recommended not only by *Nature*'s *Scientific Data* and the European Commission's *Open Research Europe*, but also by the SNSF as a repository to deposit materials-science data.

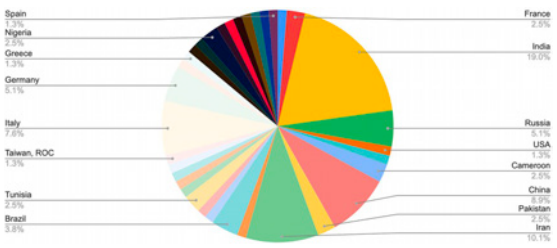

Figure 6: *AiiDA tutorial attendants nationalities.*

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, we have now provided instructions, scripts and documentation on how to deploy AiiDAlab on personal resources, from local laptops to large Kubernetes clusters (to scale to hundreds of users). Their use has been tested successfully as the computing platform for the recent AiiDA tutorials. In addition, a number of apps have been developed (see Pillar 3 and Pillar 4 sections) to cover the simulation needs of a number of MARVEL groups. 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. Details about the developments of both platforms can be found in the Pillar 3 section.

New releases, open source codes

In year 9, several new open source codes were released, with, e.g.,

- cell2mol[4], a code interpreting crystallographic files and retrieving structural, connectivity and charge information of molecules present in the unit cell (Corminboeuf group);
- Q-stack[5], a stack of codes for dedicated pre- and post-processing tasks for quantum machine learning (Corminboeuf group);

[4] github.com/lcmd-epfl/cell2mol
[5] github.com/lcmd-epfl/Q-stack

- chemiscope[6], a tool for interactive exploration of databases of materials and molecules, correlating local and global structural representations with the properties of the systems (Ceriotti group);
- Molecules[7], AiiDAlab App to compute molecular properties (Pignedoli group);
- koopmans[8], package for performing Koopmans spectral functional calculations with QUANTUM ESPRESSO (Marzari group).

Generally, open source codes developed by MARVEL researchers are listed on the MARVEL website. Tutorials are also organized to introduce these codes, e.g.

- the "Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response", online, November 9–11, with more than 200 participants and more than 800 applications, to introduce PhD students, postdocs, and junior scientists to the use of advanced functionals aimed at modeling complex materials, such as the extended Hubbard and Koopmans functionals. This tutorial was a great success based on the feedback received from the participants;
- the tutorial "Efficient materials modelling on HPC with QUANTUM ESPRESSO, Yambo and BIGDFT", online, November 14-17, with 46 participants, in which participants learned how to launch the most common types of calculations (e.g., scf, phonons, quasi-particle energies, time-dependent properties) using these codes, how to prepare input files and how to read output files in order to extract the desired properties; best practices for efficient exploitation of HPC resources were discussed, with particular emphasis on how to use the different schemes of data distribution (e.g., plane waves, pools, images) in combination with the different parallelization and acceleration schemes (MPI, OpenMP, GPU-offload) available in QUANTUM ESPRESSO.

The Psi-k 2022 conference

Presentation

The Psi-k 2022 conference, held at EPFL on August 22–25, was the 6th general conference for the worldwide Psi-k community, following very successful events held in San Sebastian (2015), Berlin (2010), and Schwäbisch Gmünd (2005, 2000, 1996).
This major conference — the largest worldwide in electronic-structure — brings together the community that is active in the field, as described by the Psi-k mission statement, "to develop fundamental theory, algorithms, and computer codes in order to understand, predict, and design materials properties and functions. Theoretical condensed matter physics, quantum chemistry, thermodynamics, and statistical mechanics form its scientific core. Applications encompass inorganic, organic and bio-materials, and cover a whole range of diverse scientific, engineering, and industrial endeavors."

Structure and key numbers

The conference program was structured around 3.5 days, that included 6 plenary talks (Fig. 7) as well as 38 symposia in 7 parallel sessions (114 invited talks and 252 contributed talks).
Initially scheduled in 2020, and postponed first to 2021, then to 2022, there was some uncertainty regarding the number of participants who would travel to Lausanne. This conference attracted an even larger audience than the previous editions: the conference received 1'269 registrations (compared to about 1'000–1'100 in the past two editions), including 21.5% of women.
The breakdown by position reveals that 29% of attendees were professors, faculties or senior researchers, 24% were postdoctoral researchers, 36% were PhD students, and another 10% were non-academic participants or otherwise did not disclose their position. Overall, attendees were working in institutions in 50 dif-

Figure 7: *Plenary talk at the Psi-k 2022 conference in Lausanne.*

[6] chemiscope.org
[7] aiidalab.github.io/aiidalab-registry/apps/empa-molecules
[8] koopmans-functionals.org/

ferent countries, with Germany, the United Kingdom, Switzerland and Italy being where half of the participants were based. A total of 82 nationalities were represented, with about 66% of participants of European nationality, and 24% of participants with nationalities in Asia (mostly India, China and South Korea), and another 9% from the Americas or Africa.
The conference involved 38 symposia, and featured 373 oral presentations (including 6 keynote speakers) as well as 717 posters.
With a total budget of 650 kCHF, this was a major event involving the entire community, including MARVEL members, which received overwhelming praise from attendees.

MARVEL contributions

The NCCR contributed significantly to the success of the conference and was deeply involved with it, driving the entire program and organization, with MARVEL director Nicola Marzari being the conference chair, and MARVEL program manager Patrick Mayor coordinating the conference organization. MARVEL furthermore contributed to the conference as an institutional sponsor.

MARVEL conference fellowships

The NCCR offered conference fellowships aiming to support groups in science that are underrepresented due to gender, ethnicity, or any other status. They were available to active PhD students or postdocs not more than two years after their PhD graduation at the time of the conference. These fellowships covered a participation to travel expenses, accommodation in Lausanne for the period of the conference, as well as the conference fees, and applicant had to propose an abstract for the conference. Out of 23 applications (22 eligible under the underrepresentation criterion), 13 were selected, all women or non-binary persons.

Best poster awards

To applaud the top posters presented by junior researchers — registered as a student or postdoc — a number of poster awards/commendations were awarded during the closing event. For each Psi-k theme (A –Physical formalisms, B – Algorithms, software and data, and C – Applications to real materials and materials design), a "best poster" prize was awarded, as well as an additional "best poster" in machine-learning-based research, each with a certificate and €150 cash prize sponsored by the Royal Society of Chemistry (Fig. 8). The winner for the machine learning award was Divya Suman (EPFL), who happens to be a MARVEL member, as a PhD student in Michele Ceriotti's group. In addition, the top 10% of posters have received a commendation, each with a €50 cash prize sponsored by Psi-k. Of the 60 commendations awarded, 10 were received by researchers involved in MARVEL.

Figure 8: *Psi-k 2022 conference: Poster awards winners. Peter Haynes, chair of Psi-k's Board of Trustees, presents the awards to Chengcheng Xiao (Imperial College London), Jennifer Coulter (Harvard University), Niamh O'Neill (University of Cambridge), Divya Suman (EPFL).*

MARVEL booth

MARVEL was present at the conference with a booth (Fig. 9) showcasing several codes, portals and services produced by its members, with live demonstrations during the lunch breaks. The participants could discover chemiscope, CP2K, SIRIUS, koopmans, IrRep, WannierBerri, AiiDA, AiiDAlab, and Materials Cloud. The Lhumos platform was presented on the adjacent CECAM booth. The INSPIRE Potentials — MARVEL Master's Fellowships were also part of the MARVEL booth with a

Figure 9: *MARVEL booth at the Psi-k 2022 conference.*

roll-up and flyers, as well as the presence, during the lunch breaks, of the MARVEL equal opportunities officer and some former and current INSPIRE Potentials fellows.

Collaborations and other conferences

Other EU and Swiss synergies

BIG-MAP Tight collaboration has been established with the H2020 BIG-MAP project, part of the Battery2030+ initiative. BIG-MAP aims at accelerating the discovery and development of novel batteries. Collaborations range from the scientific level (such as collaborations on simulations of lithium transport or open-circuit voltage), to the development of common interfaces for workflows among different codes and workflow engines (a collaboration that has been inspired by the AiiDA common workflows project discussed in Pillar 3), to the development of robust workflows (and graphical interfaces in AiiDAlab) for the prediction of spectroscopies (XPS, XAS, Raman, etc.), to technological developments: BIG-MAP developed, in collaboration with MARVEL, their internal data-sharing portal, based on a similar technology as that of the Materials Cloud *Archive* (InvenioRDM). The collaboration has also allowed the MARVEL development team to learn the features of the new version of InvenioRDM. This experience has helped to plan the technical steps needed to migrate the Materials Cloud *Archive* to the new version of the platform, that beside delivering security updates, will also provide a number of key new features to users (e.g., access with private tokens, possibility to upload larger files).

ORD initiative PREMISE A consortium led by Giovanni Pizzi, and including Carlo Pignedoli, has won funding of almost 1.3 MCHF for a three-year project dubbed PREMISE: "Open and reproducible materials science research", aimed to establish, promote and facilitate the adoption of open research data (ORD) practices that adhere to FAIR data principles in the field of materials science. The project will draw on the existing platforms openBIS, an open-source data management platform developed at ETH Zurich, and AiiDA. The two platforms focus on different parts of the data life cycle — experiments and simulations, respectively. The funding for the project is linked to the ETH Board's ORD initiative. PREMISE is an "Establish" project, meant to allow the establishment of ORD practices that already exist, bringing them to the next level, improving their scope, raising their level of quality and anchoring them as community standards.

Figure 10: *Laura Grigori (INRIA, Sorbonne University) handing the PRACE HPC Excellence award to Nicola Marzari at the PASC22 conference.*

PRACE HPC Excellence award The first-ever PRACE HPC Excellence award (Fig. 10) — a prize sum of €20'000 and a keynote slot at PASC22 conference — was awarded to N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi, and N. Marzari, for their work on "two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds", as described in their publication in *Nature Nanotechnology* **13**, 246–252 (2018). The Prize Committee highlighted that "this cornerstone work outlines the role of accurate first-principles simulations as an effective tool for materials discovery through the usage of high-performance computing. The developed digital twin of an exfoliation experiment has already had an exceptional impact in the field, leading to the discovery of new materials, in particular quantum materials."

Other collaborations In addition to the core partnerships with MaX, the EU Centre of Excellence for e-infrastructure on Materials Design at the eXascale, and BIG-MAP, the EU flagship initiative for Battery2030+, MARVEL continues benefitting from collaborations and cooperations with several European initiatives, e.g., H2020 NEP, MarketPlace, INTERSECT, DOME 4.0, or OpenModel.

Conferences organized by MARVEL members

As every years, MARVEL members organized or co-organized conferences, tutorials or workshops, with about 20 in year 9, 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.

- The CECAM workshop Quantum Transport Methods and Algorithms: From Particles to Waves Approaches, co-organized by Matthieu Luisier (ETH Zurich, July 6–8).
- The "Swiss Equivariant Learning Workshop", co-organized by MARVEL members Jigyasa Nigam and Martin Uhrin (EPFL, Lausanne, July 11–14).
- The international workshop "New Trends in Nonequilibrium Many-Body Systems: Methods and Concepts", co-organized by Philipp Werner (MPIPKS, Dresden, August 1–5.
- The symposium "Frontiers of Electronic-Structure Theory: Focus on Artificial Intelligence applied to Real Materials", co-organized by Michele Ceriotti (Regensburg, September 4–11).

5.2.2 Technology transfer

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, i.e. Frédéric Diologent (Richemont), Nicolas Cudré-Mauroux (Solvay), Thomas Eckl (Bosch GmbH), Arnaud Grandeury (Novartis), Ryoji Asahi (Toyota Central R&D Labs), and Erich Wimmer (Materials Design) as chair. Adaptations for phase III are in progress.

Industrial collaborations

Broad collaborations with Solvay, Samsung, Bosch, Gaznat, and Materials Design have started in phase II because of MARVEL, some 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.
AiiDA has been deployed by Microsoft on its Azure cloud services to run their materials searches; this close collaboration with Microsoft in continuing, and four former MARVEL members (Sebastiaan Huber, Conrad Johnston, Andrea Cepellotti and Leopold Talirz) have been hired by Microsoft. At Empa, as a collaboration with the Pignedoli group and the Laboratory of Atmospheric Modelling and Remote Sensing, AiiDA is implemented in the field of atmospheric modeling (see Pillar 4 section for the details). Collaboration with Sandvik Coromant continues, with the joint development (with the Pizzi group) of the AiiDA-LAMMPS plugin. Similarly, collaborations with SINTEF are ongoing, with SINTEF being the main maintainer of the AiiDA-VASP plugin and being involved in a number of collaborations, ranging from discussions on the features in AiiDA core, to the development of the AiiDA common workflow interfaces of Pillar 3, and their use in a scientific project for the verification of the precision of DFT simulations.

Industrial booths at the Psi-k 2022 conference

In the Psi-k 2022 conference, which was organized by MARVEL efforts, the main sponsors were given a booth in the conference exhibition hall. In additional to CECAM, MARVEL and MaX, the following industrial sponsors featured their company at the conference:

- Materials Square – a web-based materials and chemistry simulation platform;
- Microsoft, with a booth presented by former MARVEL members;
- VASP Software GmbH, which develops the Vienna *ab initio* simulation package, a leading code for quantum mechanical simulations.
- The Royal Society of Chemistry, with the three journals *Digital Discovery*, *Faraday Discussions* and *Physical Chemistry Chemical Physics*;

In addition to these booths, IBM Research Europe was also a Gold sponsor of the Psi-k 2022 conference, but opted to not hold a booth. Silver sponsors at the conference included Materials Design, Nvidia, Paul Scherrer Institute, QUANTUM ESPRESSO and Synopsys.

5.3 Equal Opportunities

5.3.1 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). The objective of phase II was to double the number of women PhD students within the NCCR, thanks to the INSPIRE Potentials Master's Fellowships, and it was achieved. In the last 2 years of phase II, more than 30% of the PhD students were women, which is still the case in year 9 (35% of women PhD students). At the other levels, the share of women postdocs remains in the low range of previous years, and the total number of senior researchers (10) is too low to be considered on a statistical aspect. If one considers the group leaders resulting from the reorganization of the phase III projects, but not the Agility Plus PIs, who are formally related to phase II, the share of women group leaders is slightly higher than at the beginning of phase II (15%, compared to 13% in year 5). This may evolve depending on the allocation of the phase III Agility Plus funding (see below).

5.3.2 Advancements of women scientists

Leadership of projects & allocation of funding

An amount of 400'000 CHF is allocated to integrate new junior and women researchers either with a call, or, more probably, direct funding to researchers identified as providing an ideal complement to an aspect of the ongoing research. The discussions are ongoing and the final decision will be taken before the end of year 9.

INSPIRE Potentials fellowships

In 2022, the flyer advertising the INSPIRE Potentials — MARVEL Master's fellowships was updated with the institutions participating in phase III. The funding opportunity was advertised as usual on Twitter and in our newsletters. In addition, from spring 2022, we started to advertise on LinkedIn and we benefitted from the enthusiasm of one of our grantees, Virginie de Mestral and a video she featured in, as a new advertising tool. Despite this, the April deadline recorded the lowest number of valid applications (3). On the other hand, the October deadline recorded the highest number (13) since the launch in 2016, perhaps thanks to the presence of advertising at the Psi-k 2022 conference. Of those applicants, one was granted the fellowship in April, and five in October. One declined because she was also selected by a doctoral school. To summarize, in addition to Mathilde Franckel, Mie Engelbrecht Jensen, and Nataliya Paulish who were already selected in 2021 and started in February and September 2022, we are happy to welcome for 6 months

- Arianna Cantarella from Univ. Parma in the group of Giovanni Pizzi at EPFL from October 2022,
- Linda Mauron from EPFL in the group of Giuseppe Carleo at EPFL from January 2023,
- Melika Honarmand from Tehran Polytechnic in the group of Michele Ceriotti from mid-January 2023,
- Noémie Hu from EPFL in the group of Berend Smit at EPFL from end of February 2023,
- Eva Doloszeski from TU Wien in the group of Sereina Riniker at ETH Zurich from September 2023 (Fig. 11).

	year 1		year 2		year 3		year 4		year 5		year 6		year 7		year 8		year 9	
	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%
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 30%	7 70%
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%	4 15%	23 85%
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%	19 35%	35 65%

Table 5.1: *Number and share of women (W) and men (M) involved in MARVEL in years 1 to 9 (From NIRA).*

Figure 11: *Top: Group picture of some former (now MARVEL PhD students) and current INSPIRE Potentials fellows at the phase II closing event; from left to right: Mathilde Franckel, Mie Engelbrecht Jensen, Chiara Cignarella, Clémence Corminboeuf, Yuri Cho, Virginie de Mestral and Lidia Favre-Quattropani. Bottom: 2022 INSPIRE Potentials fellows; from left to right: Nataliya Paulish, Arianna Cantarella, Linda Mauron, Noémie Hu, Melika Honarmand, and Eva Doloszeski.*

These students bring the number of fellowships to 42, following the 14 rounds of applications since the 2016 launch of the initiative. Of these, 12 students are already continuing or will continue at the PhD level in a MARVEL group or ex-MARVEL group. Of those who left, at least 11 are continuing at the PhD level outside MARVEL abroad. For those continuing at the PhD level in the field of MARVEL, the INSPIRE Potentials project is often crucial in the decision to stay in the domain. It is also of note that 10 former, current and future fellows were present at the Psi-k 2022 conference in August 2022 and 6 of them had an oral presentation.
Thanks to Carey Sargent, we continue to have interviews of them, as testimonials to be discovered on our website.

EPFL-WISH Foundation

In 2022, 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. 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 or workshops) organized at EPFL or in other participating institutions. Women PhD students and postdocs are encouraged to participate in training, mentoring and coaching programs offered at the various institutions.

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 9, we featured lectures from Prof. Sharon Glotzer (Univ. Michigan) and Prof. Heather Kulik (MIT), representing half of the distinguished lectures that were given. Since the beginning of the distinguished lectures series, 12 women and 20 men have participated, representing 38% women featured, which is much more than what is typical in the community — the 21.5% of women at the Psi-k 2022 conference gives a good idea of the gender distribution in the community.
An effort is also made to feature the diversity of MARVEL in the speakers presenting at the *junior seminars*, with 10 women and 14 men in the last 12 seminars, a goal that will be maintained with the relaunch of these seminars.

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.

#NCCRWomen campaign

Together with all other NCCRs, MARVEL is participating in the #NCCRWomen campaign, launched by NCCRs QSIT and Digital Fabrication, with diffusion from March until October 2021 on social media of short videos of

Figure 12: *2022 Meet the #NCCRWomen PIs of MARVEL: 2022 campaign showcasing, from left to right, Clémence Corminboeuf (photo: Alain Herzog, EPFL), Sara Bonella (photo CECAM), Ana Akrap (photo: UniFR), Sereina Riniker (photo: ETH Zurich / Giulia Marthaler), and Marta Gibert.*

women researchers, aimed at girls and women of high school or undergraduate age, in order to show what a day in the lab looks like, and why our researchers do their research. The MARVEL week, from September 27 to October 1, 2021, featured the portraits of Emiliana Fabbri (Agility Plus PI, PSI), Giuliana Materzanini (postdoc, EPFL), Chiara Ricca (postdoc, UniBE), Jigyasa Nigam (previous INSPIRE Potential fellow, PhD student, EPFL) and Miriam Pougin (PhD student, EPFL). The campaign was continued in the fall of 2022, featuring 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 channels. For Twitter, we can report 591 followers as of January 30, 2023 and an engagement (e.g., clicks, retweets, replies, follows or likes) of more than 2'000 from November 2022 until end of January 2023. 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. Notably, during the MARVEL week from November 14 to 18 we were pleased to highlight our phase III women PIs, Clémence Corminboeuf and Sara Bonella, as well as three Agility Plus PIs, Ana Akrap, Marta Gibert and Sereina Riniker (Fig. 12).

During the school year 2021–2022, some NCCRs offered high school teachers the chance to invite a woman researcher (portrayed in the campaign or not) to their class for exchanges. As the NCCRs are active in a large variety of domains, the fields proposed for these visits are as varied as mathematics, materials, linguistics, neuroscience, architecture, chemistry, robotics and microbiology. This #NCCRWomen in school, a "researcher in my class" initiative was renewed in 2022–2023. Some MARVEL researchers at EPFL visited classes in high schools in Geneva. Michele Kotiuga, in Marzari's group, visited an English class, wishing to meet a researcher whose native language is English, in May 2022, and Puck van Gerwen, in Corminboeuf's group, visited a mathematics class in January 2023; the students were very interested and asked many questions. Four other visits, also in Geneva, are already planned for the coming weeks.
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 thematic day in Thun or the lab visits during the EPFL information days for high school students. More details are given in section 5.1 on Education & Training.
These campaigns give the equal opportunities officers of the participating NCCRs a chance to meet regularly, giving them an additional occasion to share good practices and concerns.

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 year 9, two women PhD students participated in the thematic day in Thun together with a male Master student, 2 women (out of 6) supervised students during the summer camp for high school students, 2 (out of 6) for the lab visits during the EPFL information days for high school students, and 1 (out of 5) at the MARVEL stand at the 0pen doors day at PSI.

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. 13). 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 matéri-*

Figure 13: *Action for girls in 2022. From left to right:* Coding club des filles*; summer camp* Matériaux super géniaux*; chemistry summer camp; mathematics workshops* Maths en jeu*;* Polythème *workshop on materials (© EPFL SPS for all pictures).*

aux! for girls only (one in January and one in September 2022), took place on three Wednesday afternoons, and enabled participants to discover the extraordinary properties of materials. The next edition will be on February 22, March 1 and 8, 2023. The eighth edition of the summer camp *Matériaux super géniaux*, August 15–19, allowed 19 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. The next edition will be August 14–18, 2023. The chemistry summer camp for girls and boys (with 50% girls), August 8–12, 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 edition will be August 7–11, 2023.

To this, we can add the continued support of

- the mathematics workshops *Maths en jeu*;
- the *Coding club des filles*, offering coding workshops for girls 11 to 15 years old organized throughout French-, German- and now also 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.

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. As a concrete action, MARVEL has made sure the organizers of the Psi-k 2022 conference offered a daycare facility during the conference to support work-life balance of scientists who are also young parents.

5.4 Communication & Outreach

5.4.1 Internal and external communication

Website and newsletter

We continued adding to the website (nccr-marvel.ch), contributing more than 30 news items on various activities, events, awards and other news of interest to the broader community. We also wrote 21 (as of January 26, 2023) feature stories and science highlights focused on our research. We published 8 internal and scientific newsletters during the year. External readership of the scientific newsletter grew to 392 subscribers, up from 209 in January 2021 and 132 the year before.

MARVEL distinguished lectures

MARVEL has organized distinguished lectures given by prominent experts in the fields covered by the NCCR. This was originally held on site at EPFL, giving the speaker the opportunity to deliver their presentation to the local community, and was also filmed so that anyone can watch the event later on (all MARVEL distinguished lectures are made available on the *Learn* platform of Materials Cloud). The speakers also had the opportunity to have discussions and meetings with local professors during their visit. As always, and in support of equal opportunities, a specific effort was made to organize these events at 16:15, a time suitable for parents, for whom a late end might be problematic.
Since the pandemic, we have continued the distinguished lecture series in video conference mode. Trying to keep it as close as possible to the in-person experience, the events are composed of a 50-minute Zoom webinar, which is also recorded and made available on the *Learn* platform, as well as a few private online-meetings with MARVEL PIs, which we organize on or around the same day. In year 9, distinguished lectures held in this format featured

- Prof. Sharon Glotzer (Univ. Michigan), who presented "A theory of entropic bonding" on February 8, with about 130 unique viewers;
- Prof. Garnet Chan (Caltech), who presented "Is there evidence for exponential quantum advantage in quantum chemistry?" on April 5, with about 165 unique viewers;
- Prof. Alán Aspuru-Guzik (Univ. Toronto), who presented "There is no time for science as usual: Materials Acceleration Platforms" on May 31, with 200 unique viewers;
- Prof. Heather Kulik (MIT), who presented "Materials discovery in challenging spaces with machine learning: from transition metal complexes to metal-organic frameworks" on December 13. For this event, since the speaker was present for an EPFL visit at the time, we adopted a hybrid format, with the speaker delivering her presentation in a room at EPFL, welcoming about 40 attendees, and via live streaming on Zoom (with 110 unique viewers). For logistical purposes, the event was still advertised as online only, and the onsite audience was made of selected local MARVEL PIs and groups.

Since the beginning of the distinguished lectures series, 12 women and 20 men have participated.

5.4.2 Internal communication

Review and Retreats

In 2022, with the closing of phase II and the beginning of phase III, instead of organizing a September Review and Retreat event, we held two separate events in late April to formally conclude phase II and to kick off phase III.

Phase II closing event

The closing event for phase II was held on April 28 at EPFL, with more than 100 participants. Continuing a format that proved successful in recent editions, each Design & Discovery project was featured with three presentations: the project leader first presented a general overview of the main project achievements, and this was followed by two presentations given by junior researchers focused on more specific aspects of the research (Fig. 14, top). In addition, two Agility Plus projects and both Incubator projects were presented.

Phase III kick-off event

This event was organized as a half-day meeting on April 29 to introduce the main projects, as well as the various NCCR rules. The event

Figure 14: *Top: Phase II closing event. Bottom: Phase III kick-off event.*

was limited to about 30 participants, mostly the main PIs and a few collaborators. All projects' goals and objectives were presented by a project leader, and the MARVEL management team presented in detail the various NCCR management areas as well as important pointers related to open access (Fig. 14, bottom).

Year 9 Review and Retreat

Following the kick-off event in April 2022, and given that holding an event involving the whole MARVEL community in September 2023 would have been somewhat late, the NCCR decided to organize the year 9 Review and Retreat in January 2023. The event was held in Grindelwald on January 18-20, 2023, gathering all MARVEL members, group leaders as well as postdocs and students. Presentations showed the community where the projects stand and what the next steps are.
More than 100 participants joined the event (Fig. 15), which was initiated with a welcome dinner and pub quiz the first night, followed by 1.5 days of talks showcasing project achievements. Each project included a 10-minute overview presentation delivered by a project leader, followed by two 25-minute presentations by junior researchers involved in the corresponding project.
The event was widely appreciated, and we are planning to conduct our next Review and Retreat in the same location in January 2024.

Figure 15: *Group picture at the year 9 Review and Retreat.*

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.
In the original format, pizza was served before the seminar, and the participants were invited after the seminar for coffee and dessert to continue the discussion with the speakers. The organizing committee consists of delegates among PhD students and postdocs who act as chairs, with the mission to hold a lively Q&A session. The online version, started during the pandemic, limited informal interactions between participants before and after the seminars, but did have the advantage of facilitating the participation of MARVEL members from more distant locations.
In 2022, junior seminars were held until March, and April featured several junior researcher presentations at the phase II closing event. The seminars were interrupted by the buildup to the Psi-k 2022 conference, but now that we have a renewed MARVEL community for phase III, they will be launched again in a hybrid format, similar to what has been done with the distinguished lectures: seminars delivered from a special room that is well equipped for video conferences will also be streamed online, thus maintaining both the possibility of live interactions and remote access for attendees who cannot easily be present on the EPFL campus.
An effort is made to feature speakers that

represent all research areas and all MARVEL projects. In the past 12 junior seminars, 10 women and 14 men have presented their research.

Other meetings

One-to-one PI meetings with MARVEL's director

With the start of the new and last phase, Nicola Marzari, MARVEL's director, wished to meet each PI in one-to-one meetings (online or at EPFL) in October, to discuss research plans and the activities of the people of their group involved in MARVEL. Meetings with 16 PIs took place.

Projects meetings

The six scientific projects of phase III are expected to meet regularly throughout the year and the management team will help coordinate these meetings.

5.4.3 External communication

Communicating MARVEL research

EurekAlert

We continued using EurekAlert and published 11 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 were viewed more than 500 times and two, "World's largest electronic-structure conference, drawing more than 1'200 researchers, kicks off at EPFL" and "ARPES gives first observation of dispersive excitons in a low-dimensional metallic system" were viewed more than 1'000 times, according to EurekAlert statistics.

Social media

Our social media work has focused on Twitter account @nccr_marvel, which had a following of 2'027 subscribers as of January 27, 2023, up from 1'383 as of January 21, 2021. We posted an average of more than one Tweet/week over the year, earning nearly 18'000 impressions, the total tally of all the times the Tweet has been seen, and an average engagement rate, calculated as the total number of engagements (for instance, clicks, retweets, replies, follows or likes) a Tweet receives divided by the total number of views, of 4.05%. On LinkedIn, we have both a MARVEL page, with 203 followers as of January 27, 2023, where we regularly post news, and a LinkedIn group, primarily with the intention of building and reinforcing ties within the MARVEL community and keep contacts with researchers and students who have moved on.

MARVEL in web news and in the press

MARVEL research has been frequently featured on MARVEL and home institutions' websites as well as in numerous online press articles. For example, the EPFL news story "Chemical data management: an open way forward" on research from Berend Smit's group (April 2022) was featured in Sciena, Phys.org and other various websites. In November, the research from Clémence Corminboeuf's group was highlighted in news by Emily Cuffin-Munday entitled "Gigantic database of building blocks will help artificial intelligence uncover new organocatalysts" in ChemistryWorld. In June, news about the PRACE HPC Excellence Award was featured, e.g., in insideHPC or AZONANO.

Three minutes for my research

In 2022, a PhD student of the Corminboeuf group (J. T. Blaskovits) was selected for the EPFL final of "My Thesis in 180 Seconds", presenting "Fragment-based design of singlet fission materials." The challenge of this contest is to present one's research in three minutes in plain language, to a non-specialist audience. MARVEL encourages its students to participate.

Events

CECAM-MARVEL Mary Ann Mansigh conversation series

In addition to the CECAM-MARVEL "Classics in molecular and materials modeling" series, CECAM and MARVEL have initiated another events series, the "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. This series focuses on 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. The guests engage in a conversation to describe expertise, approaches to research, and career

Figure 16: *Mary Ann Mansigh conversation of Erich Wimmer with William Curtin.*

paths in this area from a perspective not usually encountered in "standard" scientific presentations.

A November 2021 event focused on the story of Olivetti's Programma 101, the world's first desktop computer. The guests for this conversation were Beniamino de' Liguori Carino (Foundation Adriano Olivetti) and Pier Paolo Perotto (Finsa, Technology for People). A May 2022 event featured Erich Wimmer, Chief Scientific Officer, and Chairman of the Board of Materials Design — as well as Chair of MARVEL's Industrial Advisory Board. He addressed the fascination and industrial value of materials modeling (Fig. 16). These events are live-streamed and recorded, ans the videos are available on Materials Cloud *Learn*. They are followed by snacks and drinks, giving attendees the opportunity to continue the conversation with the speakers.

Open doors day at PSI

On Sunday October 23, as it does every 5 years, the Paul Scherrer Institute organized an open doors day, which drew some 15'000 people. A team of five NCCR MARVEL members were present, explaining magnons and phonons and the use of supercomputers to study them to children and adults alike. The stand, "Supercomputers for Science" (Fig. 17), was sponsored by PSI's Laboratory for Materials Simulations, led by Nicola Marzari, and its Materials Software and Data group, led by Giovanni Pizzi. "Our stand was very popular and we had visitors non-stop from the beginning to the end," Flaviano Dos Santos said. "It was great to have such a close contact with people of all ages and backgrounds. It felt like we helped to inspire the next generation of scientists and engineers."

Figure 17: *Open doors day at PSI.*

Meeting with Swissnex at PSI

Swissnex has reached out to MARVEL in the context of their annual meeting, an in-person gathering bringing the Swissnex team, including the CEOs and Science Counselors, to Switzerland. During this time, Swissnex was keen to get to know the NCCR MARVEL. Members of the MARVEL management team and a few scientists traveled to PSI, where the visit took place on May 17. The main objective was to get to know the NCCR to enable potential partnerships on this domain with the Swissnex network. The program included a presentation of MARVEL Director Nicola Marzari as well as various exchanges on site and a visit of the SwissFEL facility.

Communication with the other NCCRs

MARVEL's scientific manager participated in the NCCR networking lunch organized by the NCCR TransCure in Bern on September 14. More generally, as a follow-up to the #NCCRWomen campaign and through its continuation in 2022, the NCCR management teams are developing collaborations on projects and sharing on good practices, which has been further facilitated by the establishment by the SNSF of the "NCCR network" online communication platform on Microsoft Teams, as well as the N^{ET}CC^{WO}R^{K} VENTURE funding.

5.5 Open Science

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 its scientific manager, Lidia Favre-Quattropani, and she is supported by the MARVEL data team, with in principle at least one representative per project, at disposal 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.

As requested, the MARVEL Research Data Management strategy was updated for phase III and sent to the SNSF for validation by end of May 2022. Important pointers related to open access (data and publications) were already shared with MARVEL PIs at the phase III kick-off event. 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 on nccr-marvel.ch/toolbox. In particular, one can find there the recordings and associated slides of the "MARVEL seminar on open science and open access", which took place on June 17, 2021. In October 2022, all MARVEL members received the updated RDM strategy. Finally, a session on open science was part of the Review and Retreat in Grindelwald in January 2023, announcing already the SNSF adapted open access policy as of January 2023.

5.5.2 Open access publications

MARVEL researchers know the SNSF policy concerning the openness of publications and in 2022 almost all publications (96%) are available on open access. A large half use the gold road (61 out of 110), the rest use the green road, depositing the author accepted manuscript either on an institutional repository (currently InfoScience at EPFL, DORA at PSI or Empa, Research Collection at ETH Zurich, ZORA at UZH), or a disciplinary repository (mainly arXiv.org), with apparently no journal requesting an embargo. For the five publications for which the author accepted manuscript is not available in open access, the groups have been informed that this was not compliant with the SNSF policy and that this should be taken into account for the future. All were linked with an embargo of 12 months. For one of them, the funding for open access was not anymore available for that journal, as the quota established at the national level was fully used.
The scientific manager is in contact with the EPFL library, to clarify the open access policy of some publishers. Recently, she could confirm with the American Physical Society (APS) the possibility of using arXiv.org as an open repository for their journals allowing the green road without embargo (e.g., *Physical Review B* or *Letters*). They confirmed that "posting the author-prepared version of your manuscript at any time to arXiv does not violate APS policy."
The researchers present at the MARVEL Review and Retreat in Grindelwald in January 2023 were already informed that the SNSF has adapted its open access policy as of 2023, namely that no embargos are admitted for journal articles and that a CC-BY license is requested for all articles. The entire community will be informed in the coming weeks.

5.5.3 Open data

As stated in the MARVEL RDM 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. Early May 2022, each MARVEL group was asked to make a self-assessment of its policies of data storage & backup during research, asking them about backup frequency and duration of backup retention, through an online form to be filled by the PI or someone in the group. The outcomes were good, respecting the minimal requirements of the RDM strategy, namely at least weekly backups and minimum a one-month backup retention (three-month recommended). This was also a good opportunity to inform newcomers in phase III of the expectations.
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*. Publications to the Materials Cloud *Archive* have reached the 500-mark on February 17, 2022. As Nicola Marzari said, "We are delighted to see how the community recognizes this. The first 100 records in the *Archive* took 20 months, and the last 100 only 5 months, with new submissions every day now." As of January 27, 2023, there were more than 650 entries.
For MARVEL researchers, the data underlying publications must be deposited on 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, but this also makes the data citable (with DOI), takes care of long-term preservation of the data for 10+ years, boosts visibility of the research, and increases the citation count. The use of Materials Cloud *Archive* as open repository is broadly adopted by MARVEL members. Moreover, for entries already on Materials Cloud *Archive* by mid November, we can generate the bibliography file with the related publications, asking the PIs to complete the file with the missing publications (i.e. publications with no dataset deposited on Materials Cloud or publications for which the datasets have been deposited between November and January).
MARVEL publications in 2022 generated 58 MARVEL related entries on Materials Cloud *Archive* as well as 17 entries on other open repositories. The MARVEL dataset index is available on the website, updated every year in February. 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. It is important for us to understand the reasons why authors are hesitant to put the datasets on an open repository. Finally, it should be noted that for newly submitted publications for which the preprint is available on arXiv.org, it is still compliant not to have the data in open access, and this is the case of 12 publications as of January 30, 2023.
An important recognition of MARVEL work in the domain of open research data is the funding (almost 1.3 MCHF) received from the ETH Board's ORD initiative by MARVEL PIs Giovanni Pizzi and Carlo Pignedoli for a three-year project, "Open and reproducible materials science research" (PREMISE), aimed to establish, promote and facilitate the adoption of ORD practices that adhere to FAIR data principles in the field of materials science.
Also related, a group of NCCRs, led by NCCR Microbiomes and including NCCR MARVEL, have received funding from SNSF, through the N^{ET}CC^{WO}R^{K} VENTURE to organize three joint-NCCR open research data meetings, in Zurich, Lausanne and Basel, which shoud take place between mid-April and mid June 2023.
Finally, as part as the NFFA EU project, a group of MARVEL and non-MARVEL researchers, led by Nicola Marzari, wrote a set of recommendations about good practices for data provenance, available at doi:10.5281/zenodo.7057955.

5.5.4 Open source codes

Developing codes is part of the work of MARVEL researchers, and a key aspect of MARVEL' 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 9. 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 during year 9.

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 will join EPFL in the fall of 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 is in progress as part of the third phase of the EU Centre of Excellence MaX (2022–2026).

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, 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 2022 – January 2023.

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

⬢ J. Wyzula, I. Mohelský, D. Václavková, P. Kapuscinski, M. Veis, C. Faugeras, M. Potemski, M. E. Zhitomirsky, and M. Orlita
High-Angular Momentum Excitations in Collinear Antiferromagnet $FePS_3$
Nano Letters **22**, 9741 (2022).
Group(s): Akrap / Project(s): DD6
Related datasets: not applicable

○ I. I. Mohelsky, J. Wyzula, B. Piot, G. Gu, Q. Li, A. Akrap, and M. Orlita
Temperature dependence of the energy band gap in $ZrTe_5$: implications for the topological phase
arXiv:2211.14597, to be published in Physical Review B (2022).
Group(s): Akrap / Project(s): DD6
Related datasets: not applicable

Group of Sara Bonella

⬢○ D. Du, T. J. Baird, S. Bonella, and G. Pizzi
OSSCAR, an Open Platform for Collaborative Development of Computational Tools for Education in Science
Computer Physics Communications **282**, 108546 (2023).
Group(s): Bonella, Pizzi / Project(s): P3
Related datasets: doi.org/10.17632/26py5zz9f8.1

Group of Giuseppe Carleo

⬢○ S. Barison, F. Vicentini, I. Cirac, and G. Carleo
Variational dynamics as a ground-state problem on a quantum computer
Physical Review Research **4**, 043161 (2022).
Group(s): Carleo / Project(s): QS
Related datasets: doi.org/10.24435/materialscloud:xf-wj

Group of Michele Ceriotti

⬢○ M. Ceriotti
Beyond Potentials: Integrated Machine Learning Models for Materials
MRS Bulletin **47** (2022).
Group(s): Ceriotti / Project(s): P2
Related datasets: not applicable

⬢○ R. K. Cersonsky, M. Pakhnova, E. A. Engel, and M. Ceriotti
A data-driven interpretation of the stability of organic molecular crystals

Chemical Science (2022), doi:10.1039/D2SC06198H.

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

Related datasets: doi.org/10.24435/materialscloud:71-21

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).

Group(s): Ceriotti, Emsley / Project(s): DD1

Related datasets: doi.org/10.24435/materialscloud:a9-4n

R. Fabregat, A. Fabrizio, E. A. Engel, B. Meyer, V. Juraskova, M. Ceriotti, and C. Corminboeuf
Local kernel regression and neural network approaches to the conformational landscapes of oligopeptides

Journal of Chemical Theory and Computation **18**, 1467 (2022).

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

Related datasets: doi.org/10.5281/zenodo.5172582

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).

Group(s): Ceriotti, Marzari, Pizzi / Project(s): P2, P3, P4

Related datasets: doi.org/10.24435/materialscloud:9g-k6

B. A. Helfrecht, G. Pireddu, R. Semino, S. M. Auerbach, and M. Ceriotti
Ranking the Synthesizability of Hypothetical Zeolites with the Sorting Hat

Digital Discovery **1**, 779 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:xw-5k

V. Kapil and E. A. Engel
A complete description of thermodynamic stabilities of molecular crystals

Proceedings of the National Academy of Science of the USA **119**, e2111769119 (2022).

Group(s): Ceriotti / Project(s): DD1

Related datasets: doi.org/10.24435/materialscloud:vp-jf

H. J. Kulik, T. Hammerschmidt, J. Schmidt, S. Botti, M. A. L. Marques, M. Boley, M. Scheffler, M. Todorović, P. Rinke, C. Oses, A. Smolyanyuk, S. Curtarolo, A. Tkatchenko, A. P. Bartók, S. Manzhos, M. Ihara, T. Carrington, J. Behler, O. Isayev, M. Veit, A. Grisafi, J. Nigam, M. Ceriotti, K. T. Schütt, J. Westermayr, M. Gastegger, R. J. Maurer, B. Kalita, K. Burke, R. Nagai, R. Akashi, O. Sugino, J. Hermann, F. Noé, S. Pilati, C. Draxl, M. Kuban, S. Rigamonti, M. Scheidgen, M. Esters, D. Hicks, C. Toher, P. V. Balachandran, I. Tamblyn, S. Whitelam, C. Bellinger, and L. M. Ghiringhelli
Roadmap on Machine Learning in Electronic Structure

Electronic Structure **4**, 023004 (2022).

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

Related datasets: not applicable

C. B. Mahmoud, F. Grasselli, and M. Ceriotti
Predicting hot-electron free energies from ground-state data

Physical Review B **106**, L121116 (2022).

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

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

J. Nigam, S. Pozdnyakov, G. Fraux, and M. Ceriotti
Unified Theory of Atom-Centered Representations and Message-Passing Machine-Learning Schemes

The Journal of Chemical Physics **156**, 204115 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:3f-g3

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).

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

Related datasets: not applicable

Group of Clémence Corminboeuf

R. Fabregat, A. Fabrizio, E. A. Engel, B. Meyer, V. Juraskova, M. Ceriotti, and C. Corminboeuf
Local kernel regression and neural network approaches to the conformational landscapes of oligopeptides

Journal of Chemical Theory and Computation **18**, 1467 (2022).

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

Related datasets: doi.org/10.5281/zenodo.5172582

A. Fabrizio, K. R. Briling, and C. Corminboeuf

SPA^{H}M: the spectrum of approximated Hamiltonian matrices representations

Digital Discovery **1**, 286 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:js-pz

S. Gallarati, P. van Gerwen, R. Laplaza, S. Vela, A. Fabrizio, and C. Corminboeuf

OSCAR: an extensive repository of chemically and functionally diverse organocatalysts

Chemical Science **13**, 13782 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:v4-sn

P. van Gerwen, A. Fabrizio, M. Wodrich, and C. Corminboeuf

Physics-based representations for machine learning properties of chemical reactions

Machine Learning: Science and Technology **3**, 045005 (2022).

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

Related datasets: doi.org/10.5281/zenodo.6627913

S. Vela, R. Laplaza, Y. Cho, and C. Corminboeuf

cell2mol: encoding chemistry to interpret crystallographic data

npj Computational Materials **8**, 188 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:g5-5r

Group of William Curtin

Y. Hu and W. A. Curtin

Modeling of precipitate strengthening with near-chemical accuracy: case study of Al-6xxx alloys

Acta Materialia **237**, 118144 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:9m-4n

M. Liyanage, D. Reith, V. Eyert, and W. A. Curtin

Machine learning for metallurgy V: A neural-network potential for zirconium

Physical Review Materials **6**, 063804 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:vy-02

Y. Rao, C. Baruffi, A. D. Luca, C. Leinenbach, and W. A. Curtin

Theory-guided design of high-strength, high-melting point, ductile, low-density, single-phase BCC high entropy alloys

Acta Materialia **237**, 118132 (2022).

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

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

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).

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

Related datasets: doi.org/10.24435/materialscloud:3f-w3

Group of Emiliana Fabbri

D. Hua, J. Huang, E. Fabbri, M. Rafique, and B. Song

Development of Anion Exchange Membrane Water Electrolysis and the Associated Challenges: A Review

ChemElectroChem **10** (2023).

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

Related datasets: not applicable

Group of Marta Gibert

G. De Luca, J. Spring, M. Kaviani, S. Jöhr, M. Campanini, A. Zakharova, C. Guillemard, J. Herrero-Martin, R. Erni, C. Piamonteze, M. D. Rossell, U. Aschauer, and M. Gibert

Top-Layer Engineering Reshapes Charge Transfer at Polar Oxide Interfaces

Advanced Materials **34**, 2203071 (2022).

Group(s): Gibert / Project(s): DD5

Related datasets: not applicable

Group of Jürg Hutter

A.-S. Hehn, B. Sertcan, F. Belleflamme, S. K. Chulkov, M. B. Watkins, and J. Hutter

Excited-state properties for extended systems: Efficient hybrid density functional methods.

Journal of Chemical Theory and Computation **18**, 4186 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:gw-kq

Group of Mathieu Luisier

J. Cao, S. Fiore, C. Klinkert, N. Vetsch, and M. Luisier

Light-matter interactions in van der Waals photodiodes from first principles

Physical Review B **106**, 035306 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:2z-33

J. Cao, G. Gandus, T. Agarwal, M. Luisier, and Y. Lee
Dynamics of van der Waals charge qubit in two-dimensional bilayer materials: Ab initio quantum transport and qubit measurement
Physical Review Research **4**, 043073 (2022).
Group(s): Luisier / Project(s): ASM
Related datasets: doi.org/10.24435/materialscloud:nh-nk

S. Fiore, C. Klinkert, F. Ducry, J. Backman, and M. Luisier
Influence of the hBN Dielectric Layers on the Quantum Transport Properties of MoS_2 Transistors
Materials **15**, 1062 (2022).
Group(s): Luisier / Project(s): ASM
Related datasets: doi.org/10.24435/materialscloud:7f-5t

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).
Group(s): Luisier, Passerone / Project(s): ASM
Related datasets: doi.org/10.24435/materialscloud:h4-c0

Group of Nicola Marzari

N. Biniskos, F. J. dos Santos, K. Schmalzl, S. Raymond, M. dos Santos Dias, J. Persson, N. Marzari, S. Blügel, S. Lounis, and T. Brückel
Complex magnetic structure and spin waves of the noncollinear antiferromagnet Mn_5Si_3
Physical Review B **105**, 104404 (2022).
Group(s): Marzari / Project(s): OSP, P4
Related datasets: doi.org/10.24435/materialscloud:85-ys

G. Caldarelli, M. Simoncelli, N. Marzari, F. Mauri, and L. Benfatto
Many-body Green's function approach to lattice thermal transport
Physical Review B **106**, 024312 (2022).
Group(s): Marzari / Project(s): DD3
Related datasets: not applicable

T. Chiarotti, N. Marzari, and A. Ferretti
Unified Green's function approach for spectral and thermodynamic properties from algorithmic inversion of dynamical potentials
Physical Review Research **4**, 013242 (2022).
Group(s): Marzari / Project(s): OSP
Related datasets: doi.org/10.24435/materialscloud:mx-3a

N. Colonna, R. D. Gennaro, E. Linscott, and N. Marzari
Koopmans Spectral Functionals in Periodic Boundary Conditions
Journal of Chemical Theory and Computation **18**, 5435 (2022).
Group(s): Marzari / Project(s): OSP
Related datasets: doi.org/10.24435/materialscloud:b5-8r

R. D. Gennaro, N. Colonna, E. Linscott, and N. Marzari
Bloch's theorem in orbital-density-dependent functionals: Band structures from Koopmans spectral functionals
Physical Review B **106**, 035106 (2022).
Group(s): Kenzelmann, Marzari / Project(s): OSP
Related datasets: doi.org/10.24435/materialscloud:vh-mk

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).
Group(s): Ceriotti, Marzari, Pizzi / Project(s): P2, P3, P4
Related datasets: doi.org/10.24435/materialscloud:9g-k6

T. Gorni, O. Baseggio, P. Delugas, S. Baroni, and I. Timrov
turboMagnon – A code for the simulation of spin-wave spectra using the Liouville-Lanczos approach to time-dependent density-functional perturbation theory
Computer Physics Communications **280**, 108500 (2022).
Group(s): Marzari / Project(s): OSP
Related datasets: doi.org/10.24435/materialscloud:6j-kd

M. Kotiuga, S. Halilov, B. Kozinsky, M. Fornari, N. Marzari, and G. Pizzi
Microscopic picture of paraelectric perovskites from structural prototypes
Physical Review Research **4**, L012042 (2022).
Group(s): Marzari, Pizzi / Project(s): P3,P4,OSP
Related datasets: doi.org/10.24435/materialscloud:jc-ky

S. Li, M. T. Vahdat, S. Huang, K.-J. Hsu, M. Rezaei, M. Mensi, N. Marzari, and K. V. Agrawal
Structure Evolution of Graphitic Surface upon Oxidation: Insights by Scanning Tunneling Microscopy
JACS Au **2**, 723 (2022).
Group(s): Marzari / Project(s): DD3
Related datasets: doi.org/10.24435/materialscloud:gx-se

F. Libbi, P. M. M. C. de Melo, Z. Zanolli, M. J. Verstraete, and N. Marzari

Phonon-Assisted Luminescence in Defect Centers from Many-Body Perturbation Theory

Physical Review Letters **128**, 167401 (2022).

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

Related datasets: not applicable

F. Libbi, J. Rizzo, F. Tacchino, N. Marzari, and I. Tavernelli

Effective calculation of the Green's function in the time domain on near-term quantum processors

Physical Review Research **4**, 043038 (2022).

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

Related datasets: not applicable

R. Mahajan, A. Kashyap, and I. Timrov

Pivotal Role of Intersite Hubbard Interactions in Fe-Doped α-MnO_2

The Journal of Physical Chemistry C **126**, 14353 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:8n-bm

A. Marrazzo and M. Gibertini

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

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Physical Review Research **4**, 043011 (2022).

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

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Physical Review X **12**, 041011 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:g0-yc

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Computer Physics Communications **279**, 108455 (2022).

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

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Group(s): Marzari / Project(s): INC1

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Group of Daniele Passerone

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On-surface synthesis and characterization of nitrogen-substituted undecacenes

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

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

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Group(s): Fasel,Pignedoli / Project(s): DD3

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Physical Review Research **4**, L012042 (2022).

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

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Group(s): Ceriotti, Marzari, Pizzi / Project(s): P2, P3, P4

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

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Computer Physics Communications **282**, 108546 (2023).

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

Related datasets: doi.org/10.17632/26py5zz9f8.1

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M. Thürlemann, L. Böselt, and S. Riniker

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Journal of Chemical Theory and Computation **18**, 1701 (2022).

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Group of Michael Schüler

M. Schüler, T. Schmitt, and P. Werner

Probing magnetic orbitals and Berry curvature with circular dichroism in resonant inelastic X-ray scattering

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

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

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

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Group of Ivano Tavernelli

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

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Phase II PIs, not active in phase III

Group of Ulrich Aschauer

C. Ricca and U. Aschauer

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Group(s): Aschauer / Project(s): DD5

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Group(s): Spaldin / Project(s): DD5

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Group of Urs Staub

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Group(s): Staub / Project(s): DD5

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Group of Thorsten Schmitt

A. Pietzsch, J. Niskanen, V. V. da Cruz, R. Buechner, S. Eckert, M. Fondell, R. M. Jay, X. Lu, D. McNally, T. Schmitt, and A. Foehlisch

Cuts through the manifold of molecular H_2O potential energy surfaces in liquid water at ambient conditions

Proceedings of the National Academy of Science of the USA **119**, e2118101119 (2022).

Group(s): Schmitt / Project(s): PP7

Related datasets: not applicable

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

Phase III PIs

Group of Mathieu Luisier

G. Gandus, D. Passerone, R. Stadler, M. Luisier, and A. Valli
Strongly correlated physics in organic open-shell quantum systems
arXiv:2301.00282 (2023).
Group(s): Luisier, Passerone / Project(s): ASM

Related datasets: not applicable

Group of Nicola Marzari

J. Berges, N. Girotto, T. Wehling, N. Marzari, and S. Poncé
Phonon self-energy corrections: To screen, or not to screen
arXiv:2212.11806 (2022).
Group(s): Marzari / Project(s): DD3

Related datasets: not applicable

L. Binci, M. Kotiuga, I. Timrov, and N. Marzari
Hybridization driving distortions and multiferroicity in rare-earth nickelates
arXiv:2212.12529 (2022).
Group(s): Marzari / Project(s): OSP

Related datasets: not applicable

F. J. dos Santos and N. Marzari
Fermi energy determination for advanced smearing techniques
arXiv:2212.07988 (2022).
Group(s): Marzari / Project(s): OSP, P4

Related datasets: not applicable

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
arXiv:2211.16925 (2022).
Group(s): Marzari / Project(s): P4

Related datasets: doi.org/10.24435/materialscloud:xq-5d

D. Grassano, D. Campi, A. Marrazzo, and N. Marzari
A complementary screening for quantum spin Hall insulators in 2D exfoliable materials
arXiv:2205.02583 (2022).
Group(s): Marzari / Project(s): DD3

Related datasets: doi.org/10.24435/materialscloud:z5-hm

D. Grassano, L. Binci, and N. Marzari
Prediction of a new type-I antiferromagnetic Weyl semimetal in the full-Heusler compound $InMnTi_2$
arXiv:2208.11412 (2022).
Group(s): Marzari / Project(s): DD3, OSP

Related datasets: not applicable

S. Poncé, M. Royo, M. Gibertini, N. Marzari, and M. Stengel
Drift and Hall mobility of two-dimensional materials from first principles
arXiv:2207.10187 (2022).
Group(s): Marzari / Project(s): DD3

Related datasets: not applicable

S. Poncé, M. Royo, M. Stengel, N. Marzari, and M. Gibertini
Long-range electrostatic contribution to the electron-phonon couplings and mobilities of two-dimensional materials
arXiv:2207.10190 (2022).
Group(s): Marzari / Project(s): DD3

Related datasets: not applicable

N. Rivano, N. Marzari, and T. Sohier
Infrared-active phonons in one-dimensional materials and their spectroscopic signatures
arXiv:2208.09887 (2022).
Group(s): Marzari / Project(s): DD3

Related datasets: not applicable

Y. Schubert, N. Marzari, and E. Linscott
Testing Koopmans spectral functionals on the analytically-solvable Hooke's atom
arXiv:2212.05950 (2022).
Group(s): Marzari / Project(s): OSP

Related datasets: doi.org/10.24435/materialscloud:86-bg

D. Campi, N. Mounet, M. Gibertini, G. Pizzi, and N. Marzari
Novel materials in the Materials Cloud 2D database
arXiv:2210.11301 (2022).
Group(s): Marzari, Pizzi / Project(s): P3, P4, DD3

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

Group of Daniele Passerone

G. Gandus, D. Passerone, R. Stadler, M. Luisier, and A. Valli

Strongly correlated physics in organic open-shell quantum systems

arXiv:2301.00282 (2023).

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

Related datasets: not applicable

Group of Giovanni Pizzi

D. Campi, N. Mounet, M. Gibertini, G. Pizzi, and N. Marzari

Novel materials in the Materials Cloud 2D database

arXiv:2210.11301 (2022).

Group(s): Marzari, Pizzi / Project(s): P3, P4, DD3

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

Group of Sereina Riniker

M. Thürlemann, L. Böselt, and S. Riniker

Regularized by Physics: Graph Neural Network Parametrized Potentials for the Description of Intermolecular Interactions

arXiv:2206.00355 (2022).

Group(s): Riniker / Project(s): DD1

Related datasets: doi.org/10.3929/ethz-b-000549359

Group of Philipp Werner

C. Nicholson, F. Petocchi, B. Salzman, C. Witteveen, M. Rumo, G. Kremer, F. von Rohr, P. Werner, and C. Monney

Modified interlayer stacking and insulator to correlated-metal transition driven by uniaxial strain in 1T-TaS_2

arXiv:2204.05598 (2022).

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

Related datasets: not applicable

Phase II PIs, not active in phase III

Group of Volker Roth

V. Nesterov, F. A. Torres, M. Nagy-Huber, M. Samarin, and V. Roth

Learning Invariances with Generalised Input-Convex Neural Networks

arXiv:2204.07009 (2022).

Group(s): Roth / Project(s): INC2

Related datasets: not applicable

F. A. Torres, M. M. Negri, M. Nagy-Huber, M. Samarin, and V. Roth

Mesh-free Eulerian Physics-Informed Neural Networks

arXiv:2206.01545 (2022).

Group(s): Roth / Project(s): INC2

Related datasets: not applicable

Group of Anatole von Lilienfeld

A. B. Bing Huang, O. Anatole von Lilienfeld Jaron T. Krogel

Towards DMC accuracy across chemical space with scalable Δ-QML

arXiv:2210.06430 (2022).

Group(s): VonLilienfeld / Project(s): INC2

Related datasets: doi.org/10.24435/materialscloud:p7-p8

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

J. Björk, C. Sánchez-Sánchez, Q. Chen, C. A. Pignedoli, J. Rosen, P. Ruffieux, X. Feng, A. Narita, K. Müllen, and R. Fasel
The Role of Metal Adatoms in a Surface-Assisted Cyclodehydrogenation Reaction on a Gold Surface
Angewandte Chemie International Edition **61**, e202212354 (2022).
Group(s): Fasel,Pignedoli / Project(s): DD3
Related datasets: doi.org/10.24435/materialscloud:b8-bk

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).
Group(s): Ceriotti, Emsley / Project(s): DD1
Related datasets: doi.org/10.24435/materialscloud:a9-4n

D. Du, T. J. Baird, S. Bonella, and G. Pizzi
OSSCAR, an Open Platform for Collaborative Development of Computational Tools for Education in Science
Computer Physics Communications **282**, 108546 (2023).
Group(s): Bonella, Pizzi / Project(s): P3
Related datasets: doi.org/10.17632/26py5zz9f8.1

K. Eimre, J. I. Urgel, H. Hayashi, M. D. Giovannantonio, P. Ruffieux, S. Sato, S. Otomo, Y. S. Chan, N. Aratani, D. Passerone, O. Gröning, H. Yamada, R. Fasel, and C. A. Pignedoli
On-surface synthesis and characterization of nitrogen-substituted undecacenes
Nature Communications **13**, 511 (2022).
Group(s): Fasel,Passerone,Pignedoli / Project(s): DD3
Related datasets: doi.org/10.24435/materialscloud:mc-kj

R. Fabregat, A. Fabrizio, E. A. Engel, B. Meyer, V. Juraskova, M. Ceriotti, and C. Corminboeuf
Local kernel regression and neural network approaches to the conformational landscapes of oligopeptides
Journal of Chemical Theory and Computation **18**, 1467 (2022).
Group(s): Ceriotti, Corminboeuf / Project(s): P2
Related datasets: doi.org/10.5281/zenodo.5172582

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).
Group(s): Luisier, Passerone / Project(s): ASM
Related datasets: doi.org/10.24435/materialscloud:h4-c0

R. D. Gennaro, N. Colonna, E. Linscott, and N. Marzari
Bloch's theorem in orbital-density-dependent functionals: Band structures from Koopmans spectral functionals
Physical Review B **106**, 035106 (2022).
Group(s): Kenzelmann, Marzari / Project(s): OSP
Related datasets: doi.org/10.24435/materialscloud:vh-mk

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).
Group(s): Ceriotti, Marzari, Pizzi / Project(s): P2, P3, P4
Related datasets: doi.org/10.24435/materialscloud:9g-k6

A. Kinikar, M. D. Giovannantonio, J. I. Urgel, K. Eimre, Z. Qiu, Y. Gu, E. Jin, A. Narita, X.-Y. Wang, K. Müllen, P. Ruffieux, C. A. Pignedoli, and R. Fasel
On-surface polyarylene synthesis by cycloaromatization of isopropyl substituents
Nature Synthesis **1**, 289 (2022).
Group(s): Fasel,Pignedoli / Project(s): DD3
Related datasets: doi.org/10.24435/materialscloud:yy-sc

M. Kotiuga, S. Halilov, B. Kozinsky, M. Fornari, N. Marzari, and G. Pizzi
Microscopic picture of paraelectric perovskites from structural prototypes
Physical Review Research **4**, L012042 (2022).
Group(s): Marzari, Pizzi / Project(s): P3,P4,OSP
Related datasets: doi.org/10.24435/materialscloud:jc-ky

F. Libbi, J. Rizzo, F. Tacchino, N. Marzari, and I. Tavernelli
Effective calculation of the Green's function in the time domain on near-term quantum processors
Physical Review Research **4**, 043038 (2022).
Group(s): Marzari, Tavernelli / Project(s): QS
Related datasets: not applicable

J.-Z. Ma, S.-N. Zhang, J. P. Song, Q.-S. Wu, S. A. Ekahana, M. Naamneh, M. Radovic, V. N. Strocov, S.-Y. Gao, T. Qian, H. Ding, K. He, K. Manna, C. Felser, N. C. Plumb, O. V. Yazyev, Y.-M. Xiong, and M. Shi

Giant Chern number of a Weyl nodal surface without upper limit

Physical Review B **105** (2022).

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

Related datasets: doi.org/10.24435/materialscloud:xm-dm

J. Ma, S. Nie, X. Gui, M. Naamneh, J. Jandke, C. Xi, J. Zhang, T. Shang, Y. Xiong, I. Kapon, N. Kumar, Y. Soh, D. Gosálbez-Martínez, O. V. Yazyev, W. Fan, H. Hübener, U. D. Giovannini, N. C. Plumb, M. Radovic, M. A. Sentef, W. Xie, Z. Wang, C. Mudry, M. Müller, and M. Shi

Multiple mobile excitons manifested as sidebands in quasi-one-dimensional metallic $TaSe_3$

Nature Materials **21**, 423 (2022).

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

Related datasets: doi.org/10.24435/materialscloud:sr-aa

O. Cannelli, J. Wiktor, N. Colonna, L. Leroy, M. Puppin, C. Bacellar, I. Sadykov, F. Krieg, G. Smolentsev, M. V. Kovalenko, A. Pasquarello, M. Chergui, and G. F. Mancini

Atomic-level description of thermal fluctuations in inorganic lead halide perovskites

The Journal of Physical Chemistry Letters **13**, 3382 (2022).

Group(s): Kenzelmann, Pasquarello / Project(s): DD3, OSP

Related datasets: doi.org/10.5281/zenodo.6394065

F. Petocchi, C. Nicholson, B. Salzmann, D. Pasquier, O. Yazyev, C. Monney, and P. Werner

Mott versus Hybridization Gap in the Low-Temperature Phase of 1T-TaS_2

Physical Review Letters **129**, 016402 (2022).

Group(s): Werner, Yazyev / Project(s): ASM, DD5, DD6

Related datasets: doi.org/10.24435/materialscloud:v6-nk

J. Rizzo, F. Libbi, F. Tacchino, P. J. Ollitrault, N. Marzari, and I. Tavernelli

One-particle Green's functions from the quantum equation of motion algorithm

Physical Review Research **4**, 043011 (2022).

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

Related datasets: not applicable

M. Schüler, T. Schmitt, and P. Werner

Probing magnetic orbitals and Berry curvature with circular dichroism in resonant inelastic X-ray scattering

npj Quantum Materials **8**, 6 (2023).

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

Related datasets: doi.org/10.24435/materialscloud:ck-7m

S. Wang, T. Nishiuchi, C. A. Pignedoli, X. Yao, M. Di Giovannantonio, Y. Zhao, A. Narita, X. Feng, K. Müllen, P. Ruffieux, and R. Fasel

Steering on-surface reactions through molecular steric hindrance and molecule-substrate van der Waals interactions

Quantum Frontiers **1**, 23 (2022).

Group(s): Fasel, Pignedoli / Project(s): DD3

Related datasets: doi.org/10.24435/materialscloud:d7-kq

Cover picture

Schematics of a photo-detector based on a $MoSe_2$-WSe_2 van der Waals heterostructure. Light coming from the top is absorbed in one of the two 2D materials or across them. This process generates electron-hole pairs that are separated and collected in both device electrodes (group of Mathieu Luisier, ETH Zurich).

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