MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Materials' Revolution: Computational Design and Discovery of Novel Materials

Progress Report

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Wildhainweg 3, P.O. Box 8232, CH-3001 Berne

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NCCR Director / Co-Director Name(s), first name(s) Institution(s)	 Nicola Marzari EPFL
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Contents

1 Executive summary

MARVEL is close to completing its 7^{th} year, with phase 2 in full swing (the themes for phase 1 being "Building Community and Tools" and phase 2 "Design and Discovery of Novel Materials"). The core objective of any NCCR is that of igniting collaborative research with long-term structural impact, and this becomes very apparent in the pages that follow — from the reports on the research projects, the open-science platform, the management activities, and the highlights below. The numbers help also frame the entire effort: MARVEL community has had 12 active ERC grants in phase 2 (22 in total), and produced 198 papers in year 7, of which 116 with direct support from MARVEL funding. Moreover, 186 of these papers are published under open-access protocols, and 95 open-access datasets, mostly on the Materials Cloud *Archive*, are also made available. For the first 3 years of phase 2, 497 MARVEL papers have been published in total, of which 281 with direct support, and 135 as inter-group or inter-project collaborations.

D&D1 Molecular materials, e.g., those formed by pharmaceutical compounds, pose formidable modeling challenges. This D&D project has developed, demonstrated, and distributed breakthrough simulation techniques, powered by accurate quantum computations, advanced statistical sampling and machine learning models, to address these challenges, increasing the predictive power of phase space exploration and complex properties and bringing together computation and experiments.

D&D2 This project has now developed a robust, efficient library for atomic-scale machine learning, has demonstrated that machine learning potentials enable study of complex metallurgical phenomena in alloys, has progressed toward linking across scales in metallurgical performance, and has made significant advances to the first-principles-based prediction and design of high entropy alloys.

D&D3 This project is dedicated to the design, discovery and engineering of low-dimensional materials and nanostructures. Here, the portfolio of inorganics materials has now reached $\sim$ 3500 different materials, leading to the prediction of the highest superconducting temperature for a 2D monolayer (21–27 K in W_2N_3) and the identification of optimal 2D monolayers for ultra-scaled field-effect transistors, with ON-state currents outperforming most transition-metal dichalcogenides. The nanostructure design has had a number of major accomplishments, including the demonstration of unconventional magnetism in nanoribbons, engineered with the simulations to be topologically frustrated.

D&D4 This project aims to develop and apply computational method to better understand the properties of metal organic frameworks (MOFs). An important aim for phase 2 in MARVEL is to demonstrate that computational materials design can result in novel materials. In D&D4 we now have three examples in which novel computationally designed materials were subsequently synthesized. These examples are related to fundamental questions on how to tune the optical and electronic properties of MOFs. A major breakthrough was achieved to design novel materials for carbon capture. A key challenge was to find a material that can capture CO_2 in wet flue gasses. The material that was discovered computationally and subsequently synthesized in D&D4 outperformed commercial materials.

D&D5 Our project is building fundamental understanding of correlated oxides to enable guided computational design of new correlated materials with specific targeted functionalities. We develop the methodologies required for predicting the properties of correlated oxides, incorporate them into publicly available codes, and apply them to materials design, focussing in particular on the interplay between chemistry, dimensionality, defect chemistry and properties.

D&D6 This project aims at the discovery of novel topological materials with the ultimate goal of realizing practical applications of this

diverse class of emerging systems. Among numerous achievements during phase 2 the following stand out: (i) extension of topological classification with the non-Abelian band topology; (ii) discovery of novel graphene moiré superlattice systems; (iii) a series of experimental works aiming at validating theoretical predictions, e.g., the confirmation of the Weyl semimetal phase in β-WP_2.

Inc1 This project is a synergistic project relying on continuous feedback between theory and experiment to accelerate the discovery of novel solid-state electrolytes with improved ionic conductivity, wide electrochemical stability window, and favorable mechanical properties. So far, we developed and made available through AiiDA three computational tools (screening method, stability tool, neural-network architecture), wrote an extensive review on experimental methods for microbatteries, and identified five technologically relevant electrolyte materials.

Inc2 Within this project, research deals with improving machine learning procedures applicable to the problem of computational materials design. Published activities included improved representations and inverse learning of symmetries. Codes and documentations, as well as work on non-covalent interactions (see D&D1), have been contributed as well.

OSP The Open Science Platform represents the core structural effort of MARVEL, to develop a world-class computational facility: an infrastructure, based on AiiDA, where multiple simulation services are offered, from fail-safe "turnkey" materials-science workflows to new methods for computational spectroscopies and microscopies. AiiDAlab makes these capabilities available on the cloud, and the Materials Cloud portal enables dissemination and FAIR sharing of these results in an Open Science model. All these activities have now major demonstrators in place, notably also the AiiDAlab apps for automated QUANTUM ESPRESSO simulations, and to probe any computational database complying with the OptiMaDe universal REST API.

HPC The HPC platform continued to operate smoothly, delivering the infrastructure as a service, needed for the deployment of the Materials Cloud platform. These services are essential for the MARVEL project. The software efforts have lead to the SIRIUS library that is available to all CSCS users, that is fully validated, and that is enhanced for the high throughput calculations typical of MARVEL workflows. In particular, the SCF success rate has increased from 90% to 99.5+% for challenging magnetic systems. Furthermore, this software has been ported from Nvidia to AMD GPUs, guaranteeing readiness of key MARVEL codes on European and US (pre-)exascale architectures.

Structure-related aspects The tech transfer activities have seen the very successful completion of the 5 industry sector days, engaging 45 companies in MARVEL research; a start-up from MARVEL students is also incubating. The MARVEL distinguished lectures and the CECAM-MARVEL Classics in molecular and materials modeling have gone fully online, reaching an even broader audience. In equal opportunities, 4 junior women PIs have joined MARVEL, supported by the new Agility Plus funding.

2 Reaction to the recommendations of the review panel

The feedback from the review panel was overall very positive. We report here representative excerpts, mentioning that

"The scientific work of MARVEL continues to be of a very high standard. Both breadth and the quality of the science covered by the NCCR is truly stunning. Of course it is a large group, with enormous expertise in many areas of computational materials science, but it is impressive because many well established groups (who most likely did not need to collaborate) have nevertheless come together and found fruitful ways to work in a common framework and add value. Their research has clearly benefitted from the development of MARVEL, allowing many PI and research groups to extend their research activities in new directions."

"The scientific output of the MARVEL groups has continued to be at the highest level, in terms of both quality and quantity, as shown by the large number of publications in prestigious journals. New materials with desirable properties have been identified, new methodologies have been developed, and codes have been written and placed in the public domain. Several of the efforts are world-leading. There are breakthroughs, such as discovery of new 2D materials with unexpected properties in D&D3, identification of materials with new topological properties in D&D6, development of new physically-inspired machine learning methods in D&D1, and the application of these methods to solve long-standing problems in atomistic modelling in Incubator 2."

"In short: MARVEL has clearly become a world-class research programme."

We present below a response to the questions asked or to the points raised.

1 Response to the reaction to the panel recommendations

The efforts and measures on the gender equality issues were recognized and highly appreciated by the panel. They also acknowledged the significant increase in the number of female PhD students.

Regarding machine learning, the panel regrets that *"the expertise of D&D Project 1 has not been taken to many of the other projects (D&D2 is a notable exception) . It is pointless predicting new materials or devices if these cannot be fabricated or suffer a larger scale failure mechanism — topics that can begin to be addressed by the methods developed in D&D1."* The panel also says in its main recommendations that *"There must be a greater emphasis on using the theoretical tools to help design fabrication routes and test for failure modes of materials and devices."*

This recommendation, with which we fully agree, lies at the foundation of Pillar II for phase 3, where the methods developed in D&D1 will build and disseminate the machine-learning infrastructure to the broader MARVEL community. It should also be noted that machine-learning efforts are present in many other projects, when relevant — D&D3 to predict exfoliability, D&D4 for gas storage and separation, and Inc1 for accelerated molecular dynamics. At the same time, we also underscore that testing for failure modes can be (in many but not all cases) exceedingly hard.

The positive feedback of the panel regarding the efforts of MARVEL to increase its interaction with industry is appreciated and recent developments in year 7 can be found in the technology transfer section.

Finally, we take note of the requirement to provide a spreadsheet detailing the activities of the different PIs in the management areas. We will prepare it for the forthcoming site visit.

"The concern is that the main effort involved in these activities is being carried by a relatively small number of MARVEL personnel."

While this might be true for some of the senior investigators, there is also a very driven and energetic community of young PIs that will be at the core of phase 3 and the post-2026 long-term effort. Also, the engagement of the junior scientists and students has been outstanding.

2 Response to scientific performance

The report mentions that *"both breadth and the quality of the science covered by the NCCR is truly stunning"* and that the PIs' *"research has clearly benefitted from the development of MARVEL, al-*

lowing many PI and research groups to extend their research activities in new directions", "in short: MARVEL has clearly become a world-class research programme". The review panel acknowledges the added value brought by our NCCR, which is a recognition that is very encouraging at the time of preparing the pre-proposal for the next 4-year period.

3 Response to internal collaboration and synergies

The panel notes the high rate of collaboration and synergies within the NCCR, between the PIs within a project, *"and in many cases, the PIs collaborate across the various projects, leading to stronger cohesion in the center, and also stronger scientific impact".* The anchoring on the developments of phase 1 is raised. However *"The panel would like to see more of such multi-team collaborations within MARVEL"* and *"a few groups, while being world leaders in their field, seem to have almost no interaction with the other MARVEL groups — at least as far as one can judge based on the absence of joint publications. It is possible that synergies exist without joint publications resulting from them."*

Indeed quite often some of these key synergies exist even if not directly testified by an immediate joint publication. Notable examples are the developments of the CP2K and SIRIUS codes, that are of utmost importance for the calculations in many projects, but still do not necessarily lead to frequent joint publications.

"Some reviewers have the impression that the MARVEL effort has split into two tracks: those who are doing high throughput/machine learning, and those who are doing more conventional method development, and there seems to be little crosstalk between these two tracks. However, most groups seem to be contributing to joint efforts such as the AiiDA platform and the Materials Cloud."

High-throughput, machine learning, and method development are some of the strongest present or historical strengths of this community — we do not, however, see separate tracks and there are and have been many stimulating interactions — as an example, some of the state-of-the-art approaches of the Werner group on nickelates, combining GW and EDMFT, provide the reference results to explore more approximate approaches based on single-site DMFT in the Ederer group and on extended Hubbard functionals in the Marzari group.

In its main recommendations, the panel suggests that *"the NCCR should continue to promote multi-team collaborations, and further encourage or provide bonuses for collaborative efforts between groups with different expertise."*

We are actively doing this, and many collaborations are very lively and active — last but not least with also the many experimental groups that have been engaged. The current budget does not allow us to allocate additional bonuses without cutting support elsewhere, but we feel that the portfolio of activities is healthy and balanced.

4 Response to international standing

We thank the panel for the very positive evaluation of the effort.

5 Response to knowledge and technology transfer / Public outreach and communication

We thank the panel for the positive comments; activities will continue strongly in this.

6 Response to education and training

"The education and training activities within MARVEL have a remarkable emphasis on the role of PhD students and young scientists, including junior seminars, which were already organized in the previous years, and a summer school organized exclusively by four PhD students held at EPFL." "All the evidence points to high levels of satisfaction among the young researchers (PhD, postdocs). They are provided high quality mentoring and opportunities for collaboration, but they also have the possibility to take their own initiatives."

The recognition of students' involvement in the implementation of activities for themselves is very much appreciated and encourages us greatly in this process, which allows students not only to be trained in their research fields and but also in soft skills. As mentioned earlier, the enthusiastic participation and response from the young researchers has been one of the most rewarding results of our efforts.

7 Response to equal opportunities

We greatly appreciate that *"the panel applauds our efforts to date, but also encourages us to diligently continue our hard work in this area."* The section of the report on equal opportunities shows that we have continued along this path this year with the launch of the Agility Plus projects and the subsequent hiring of PhD students in four groups led by female PIs, granting (a few) INSPIRE Potentials fellowships despite the difficulties raised by the COVID-19 pandemic, and maintaining all the activities

for girls with the requested sanitary measures. The challenge of increasing the share of women in MARVEL indeed remains one of the hardest and we appreciate the positive note of the panel: *"It must be recognized that in the general field of this NCCR the number of female researchers globally is very low, and there is only a limited amount that can be done to raise the numbers in the short term. Within this global constraint, the initiatives of this NCCR are exemplary."*
"The panel is pleased to hear that the training sessions on gender and diversity awareness were quite successful and well received. Not all of the MARVEL PIs participated and for the student training session, not all groups were represented. In some cases the reason seems to have been conflicting commitments. The panel suggests integrating these offers into other MARVEL activities such as retreats or scientific workshops. They will then have to be shorter, but are perhaps more likely to have greater participation."
We are indeed convinced of the importance of awareness training for gender bias and fully intend to continue these efforts. We took note of the suggestion to integrate such an offer into other MARVEL activities, such as retreats or workshops — something we will act on as soon as live activities restart.

8 Response to structural aspects

The search for a new tenure-track assistant professor in computational materials science is ongoing, with interviews of 11 shortlisted candidates scheduled between February 22 and March 5, 2021. The position should lead to an appointment in the fall and will certainly have key impact in the remaining years of the NCCR. MARVEL funding has also been allocated to rapidly integrate the new group.

9 Response to recommendations

"The main recommendations by the panel can be summarized as follows:

- *The NCCR should continue to promote multi-team collaborations, and further encourage or provide bonuses for collaborative efforts between groups with different expertise.*

  This remains a core focus for the project, and it is also evident in the Annex list of collaborative publications. The "horizontal" efforts driven by the MARVEL codes, AiiDA and the Materials Cloud, the machine-learning infrastructure will also keep driving these synergies.

- *There must be a greater emphasis on using the theoretical tools to help design fabrication routes and test for failure modes of materials and devices.*

  Theoretical tools and machine learning efforts for synthesis (e.g. the nanoporous materials) or synthesis (e.g. metal alloys) are very much in place. Failure modes, as mentioned, are very complex, but an ongoing collaboration at the automated calculations of defect formation energies, dopants, and interstitials in any charge state will provide a very robust baseline to understand the resilience of materials and their properties against defects.

- *The panel suggests integrating gender awareness trainings into other MARVEL activities such as retreats or scientific workshops. They will then have to be shorter, but are perhaps more likely to have greater participation.*

  We are fully in agreement and dedicated to this.

- *For the preparation of phase 3, the panel would not recommend linear cuts for all projects, but rather selective decisions, focusing on achievements which are only possible in the NCCR context and on efforts helping to sustain the NCCR's impact after its end. The panel is ready to comment on phase 3 plans before the submission of the elaborated pre-proposal if the NCCR directorate thinks this is helpful (e.g. in autumn).*

  Indeed, our concept presented to the panel in November, and the pre-proposal are fully aligned with these recommendations, and received very positive feedback also from the Scientific Advisory Board.

- *The panel would like to receive a similar overview detailing the activities of the different PIs for center-related goals such as education, outreach or technology transfer as distributed in year 4 every year now."*

  Certainly. This overview will be provided in advance of the site visit.

3 NCCR Organisation

3.1 Structure and organisation of the NCCR, management activities

3.1.1 Structure of the NCCR

In phase 2, MARVEL is organized around 6 Design & Discovery projects (major collaborative projects covering key topics in energy, ICT, manufacturing, chemistry and pharma, and ranging from molecular crystals to complex metal alloys to topological materials), 2 Incubator projects (more focused efforts, dedicated presently to solid-state ionic conductors and machine learning). In addition, 2 core structural efforts are represented by the Open Science platform (which provides open access to simulation services and tools, dissemination and preservation of curated and raw data, and educational material) and the HPC and Future Architectures platform, which supports the deployment of the next hardware resources for MARVEL, and the co-design of software and hardware (Fig. 1). EPFL is the home institution and participating scientists are affiliated with 11 Swiss academic and industrial institutions.

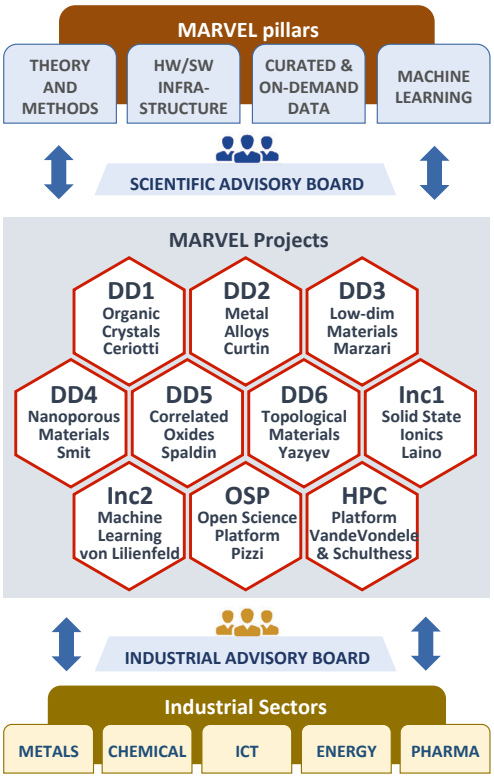

Figure 1: *Structure of NCCR MARVEL in phase 2.*

In phase 2, along with the director, Nicola Marzari, Berend Smit (EPFL) is deputy director, and Clémence Corminboeuf (EPFL) and William Curtin (EPFL) complete the Executive Committee in charge of day-to-day activities.

Strategic decisions (reallocation of funding, establishment and termination of projects) are taken by an enlarged committee, the Strategic Committee, which was slightly reorganized in year 6, including, in addition to the Executive Committee, Thomas Schulthess (CSCS and ETHZ), Frithjof Nolting (representative of PSI) and Daniele Passerone (representative of Empa).

Finally the Scientific Committee is composed of the Strategic Committee and all project leaders; it has the formal role of discussing the science and an advisory role on strategy.

A Scientific Advisory Board (SAB) of nine members, chaired by Giulia Galli (Univ. Chicago), and an Industrial Advisory Board (IAB) of six members, chaired by Erich Wimmer (Mat. Design), provide feedback on all activities and convene once a year (SAB, at the Review and Retreat) and one every two years (IAB).

3.1.2 Organisation of the NCCR

Six new members entered MARVEL in May 2020. Lyndon Emsley (EPFL) joined the D&D1 project as experimental PI through some reallocation of funding within the project and Urs

Staub (PSI) joined D&D5 for the second half of the phase, replacing Marisa Medarde (PSI) as already planned in the proposal for phase 2. Moreover, four new female PIs, Sereina Riniker (ETHZ) in D&D1, Emiliana Fabbri (PSI) in D&D4, Marta Gibert (UZH) in D&D5 and Ana Akrap (UniFR) in D&D6, joined MARVEL through the Agility Plus call for projects. Marisa Medarde's project, planned only for the first half of the phase, carried over the first three months of year 7 until the end of July and Michele Parrinello retired at the end of December 2020.
Within the management team, Carey Sargent reduced her activity rate from 40% to 20% since May 2020, activity rate taken over by Patrick Mayor, going from 60% to 80%. Pascale Van Landuyt left her role at 20% as MARVEL industrial liaison and tech transfer officer at the end of November 2020, taking other responsibilities at EPFL. Her replacement is under discussion. The MARVEL data team also underwent some changes and replacements were made in order to broadly represent the different projects and institutions (nccr-marvel.ch/people/governance/data-team).

3.1.3 Activities and measures

Events organisation

In year 7, despite of the COVID-19 crisis, MARVEL management nonetheless organized meetings, lectures and events, described in chapter 5. We mention, for example:

- Meeting of the MARVEL Industrial Advisory Board (IAB) at EPFL, February 6.
- Panel Discussion: "Scientific research in industry: What you want to know" with the IAB, February 6.
- MARVEL stand at International Women's Day "Shoot for the Moon", EPFL, March 5.
- Online site visit, April 23–24.
- Online meeting of the MARVEL data team, May 28.
- Online Strategic Committee Meeting, July 16.
- Online MARVEL Review and Retreat, September 10–11.
- INSPIRE Potentials — MARVEL Master's Fellowships for female Master's students, with 2 calls in April and October.
- 1 Industry Sector Day at EPFL, on materials for energy, February 7; 2 online Industry Sector Days, on materials for electronics, December 4, and chemistry & catalysis, January 14.
- MatScreen team support by MARVEL TT officer.
- 2 online MARVEL distinguished lectures, Stefano Baroni (SISSA,Trieste), November 17, and Silvia Picozzi (CNR-SPIN, Chieti), December 15.
- 1 junior seminar at EPFL in February; 7 online junior seminars since May, continuing on a monthly basis.
- 3 seminars at EPFL, before partial lockdown in March.

Some events, turning online, did no longer request the assistance of the MARVEL management as, e.g., the virtual edition of the AiiDA introductory tutorial, July 7–10. Other events were cancelled, but nevertheless occupied the management team, for example:

- The MARVEL stand at the EPFL Industry Day, planned March 25.
- The Ig Nobel Award Tour Show at EPFL, planned March 30.
- The summer camp for high school students *Des atomes aux ordinateurs, à la découverte de la programmation scientifique* at EPFL, planned June 29 – July 3.

Other events

In year 7, MARVEL members organized 10 conferences, tutorials or workshops (not counting AiiDA tutorials), most online. Since the beginning of phase 2, this list goes up to about 50 (nccr-marvel.ch/ctw), of which MARVEL sponsored 13.

Measures

The management team has prepared a "Welcome Letter" with information and requirements regarding finances, acknowledging MARVEL in publications, visual identity, equal opportunities and tech transfer themes. It has been sent to all MARVEL members in January 2019 and has been updated to reflect new rules or personnel.

Research data management

Day to day work data are either stored on local group resources under the responsibility of the researchers/PIs or on the MARVEL-supported /store partition at CSCS. In March 2020, as stated in the MARVEL research data management (RDM) strategy, each MARVEL group was asked to make the annual 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 globally good, respecting the minimal requirements of the RDM strategy. Non-complying groups were informed through the MARVEL data team, whose role is to be the point of contact, to raise awareness on data

management and to check the minimal requirements presented in the MARVEL RDM strategy.
MARVEL publications in 2020 generated about 85 MARVEL related entries on Materials Cloud *Archive* as well as some entries on other open repositories, compared to 70 in 2019, and 163 since the beginning of the repository. The MARVEL dataset index is available on the website on nccr-marvel.ch/publications/dataset-index and in a printed version in the Annex 2 of this report. 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). 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 do not. It is important for us to understand the reasons why authors are hesitant to put the datasets on an open repository, in particular in view of the update of the MARVEL RDM strategy for the full proposal in September 2021.
Also related to publications is the openness of the publications themselves. The policy of the SNSF is known by the researchers and in 2020 almost all publications (94%) are available on open access. The few missing are most of the time linked with an embargo of more than 6 months, and 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. As already mentioned last year, in the physics side of the community, the preprint server arXiv.org has already been well implemented for a long time. Now most of the institutional repositories (InfoScience at EPFL, DORA at PSI and Empa, Research Collection at ETHZ, edoc at UniBas, etc.) manage by themselves the embargo, giving already at the time of publication an open access link that will allow free access to the publication at the end of the embargo, releasing the responsibility of the authors to come back later.
Both aspects, data management and open publications, have been treated on the website and relayed through the internal newsletter to widely inform MARVEL members. Moreover we will organize early spring one seminar for the junior researchers on how to comply to open access publication policies and open access data.

3.2 Status of collaboration/integration, added value

3.2.1 Status of collaborations and integration

At the NCCR level

All projects in phase 2 are intensely collaborative, with a project leader integrating the different computational efforts of the co-PIs, and in most cases including funded or matching experimental efforts. It is only because of MARVEL that these projects were nucleated and grown, and the ongoing close interest and support taking place at CSCS, PSI and Empa reassure us of the long-term effects and collaborations that these projects are establishing. Having a common hardware and software infrastructure deployed at CSCS, a data infrastructure in the Materials Cloud, and an operating system with AiiDA make MARVEL a think tank and a working laboratory to develop the vision, synergies and facilities/infrastructure for computational science.

At the national level

The integration efforts of MARVEL are very notable both between the community of PIs, encompassing all groups in computational condensed-matter physics and materials science, and many of those in chemistry, and in terms of integration within the national laboratories (PSI and Empa). These latter two, together with CSCS, provide the long-term support for the vision of MARVEL to be established in the national landscape.

At the international level

Many international and European projects are active in MARVEL (including 12 ERC in phase 2), but most notable for the long-term establishment are the partnership with

- MaX, the H2020 Centre of Excellence for eInfrastructure (2015–2018, 2018–2021,

tbd) with strategic partnerships on HPC, HTC, co-design, and the Materials Cloud
- BIG-MAP, a core effort in the 10-year Battery 2030+ initiative, where MARVEL and CSCS provide core infrastructure for data storage and simulation services
- the H2020 projects driven by the EMMC-CSA, with MarketPlace, Intersect, DOME 4.0 and OpenModel dedicated to integrating simulations in the European industrial landscape
- CECAM, with which MARVEL has established a long-term plan of dissemination and educational activities

3.2.2 Added value

The ecosystem of codes (from CP2K to SIRIUS to QUANTUM ESPRESSO to correlated electrons to machine-learning), the integration in AiiDA and AiiDAlab, the dissemination of data and simulations through the Materials Cloud would not exist or would not be at the present state of development without MARVEL — this will be core to the long-term sustainability of the community in Switzerland.

3.3 Impact of the COVID-19 pandemic

The COVID-19 pandemic and the consequent worldwide social restrictions have posed unprecedented challenges to the scientific community. Although MARVEL-related institutions and MARVEL groups reacted very well on a remote-working basis — the advantage of computational research — there were still intrinsic limitations, mainly in the education, knowledge transfer and communication areas. As a result, many activities that we planned to organize or to participate in could not happen. Nonetheless, some took place, many were transferred online, and others still were created for the occasion. A consequence also was less spending, as an online event does not need to provide coffee breaks or lunches.
Another impact of the pandemic is some delay in hiring processes, in particular for the new Agility Plus PIs, starting in May 2020. We noticed that we received fewer applications for the INSPIRE Potentials Master's fellowships, with also a higher proportion of "local" applicants — already studying in a Swiss university part of the MARVEL network — due to travelling difficulties. Even if computational research is less impacted by remote-working than lab research, keeping the distant supervision and coaching close to the students (in particular the Master's students, as the INSPIRE Potentials fellows), especially at the beginning of a project, was a challenge, and the personal engagement of all supervisors is acknowledged. As mentioned in the equal opportunities section, remote work may have amplified some differences between students, shy students sometimes less proactive on Zoom and benefitting less from the group dynamic.

4 Research

4.1 Results over the past 33 month

Design & Discovery 1 — Understanding Complex Molecular Crystals: Structure and Properties

Project leader: Michele Ceriotti (EPFL, 1MC)

Computational partners: Clémence Corminboeuf (EPFL, 2MC), **Stefan Goedecker** (UniBas, 1MC), **Michele Parrinello** (USI and ETHZ, 1MC), Anatole von Lilienfeld (UniBas), **Sereina Riniker** (ETHZ, Agility Plus, 0.8MC)
Experimental partners: Esther Amstad (EPFL), **Lyndon Emsley** (EPFL, 0.5MC)

This D&D project addresses the modeling challenges connected with the computational description of molecular materials, particularly those composed of large, flexible units. Over the past 33 months, the team has successfully tackled multiple aspects of the problem, including the search for conformers and crystalline polymorphs, the prediction of stability and properties of different phases, and the modeling of the crystallization process.

1 Progress of the different efforts

1.1 Anharmonic and quantum free energies

Proof-of-principle work during phase 1 revealed the importance of finite-temperature and quantum mechanical fluctuations of the nuclei for determining stability and properties of molecular materials, but also the enormous cost of incorporating these effects with first-principles energetics [1]. We have therefore implemented in i-PI [2] several methods to approximate anharmonic free energies, and benchmarked them on different classes of materials [3]. Despite the promising accuracy of these methods for typical inorganic materials (a result that could be of great use for MARVEL at large) this work showed that the type of anharmonicities occurring in molecular compounds require a fully anharmonic treatment. We are thus exploring complementary approaches, relying heavily on machine-learning (ML) models, but also on their interplay with enhanced sampling methods such as replica exchange and metadynamics, to achieve statistically converged thermodynamic properties of flexible molecules at high *ab initio* level [4, 5].

1.2 Molecular conformers and crystal structure search

Thanks to a built-in feedback mechanism discouraging oversampling regions of phase space that have already been visited, minima hopping is an ideal tool to study complex conformational landscapes off molecules and their packing [33]. The introduction of a permutation-invariant bias further improves this approach by making it possible to pull the system towards a specified end state, thereby identifying complex transformation pathways between different structures. Although initially developed for molecules [6], this method has been extended to treat periodic systems, and to help understanding whether theoretical structures can be grown experimentally or whether their formation is kinetically suppressed [7]. The group of Sereina Riniker — who recently joined the collaboration on an Agility Plus grant — is currently work-

ing to use Bayesian neural networks to restrict the search space for the most stable polymorphs, and to use simulations of molecular compounds in the molten phase to determine the conformers that are most likely to be found in the crystalline phase — which often differ from those obtained in a gas-phase search.

1.3 Interface energies and nucleation kinetics

Nucleation is a crucial process to understand the stability of molecular materials, because it often determines the formation of metastable phases, due to kinetic trapping. Studying nucleation by atomistic simulations is a challenge due to the enormous gap separating the time scale of atomic motion and that of an activated phase transition. The development of more effective approaches to bias simulations to overcome this time scale issue has been a very successful endeavor connected to this project. For example, the on-the-fly probability enhanced sampling (OPES) provides a novel unified perspective on enhanced sampling, allowing for a replica-exchange-like sampling within a collective-variable-based method [8, 9], thereby making enhanced sampling more accessible and efficient, and more easily applicable to complex materials. Liquid Ga provides a test bed to demonstrate how these techniques can address many of the challenges inherent in molecular materials, revealing the mechanism by which, at low temperatures, the formation of metastable β-Ga is kinetically favored over the thermodynamically stable α-Ga [10] (Fig. 1).

Other methods have also been developed that tackle challenges that are specific to the nucleation of molecular compounds, such as the realization of constant chemical potential molecular dynamics (CμMD) that maintain a realistic level of supersaturation with an affordable simulation size [11]. CμMD has been applied to study solvent-dependent morphology selection of an anti-tuberculosis drug, isoniazid [12], and supersaturation-dependent crystal shape prediction of naphthalene in ethanol solution [13]. A spherical variant of the CμMD has been developed to study homogeneous nucleation from solution [14].

1.4 Machine learning for molecular crystals

The need to obtain accurate energetics together with extensive thermodynamic sampling has triggered an extensive effort in the development of machine-learning techniques. While focused on problem of interest for molecular

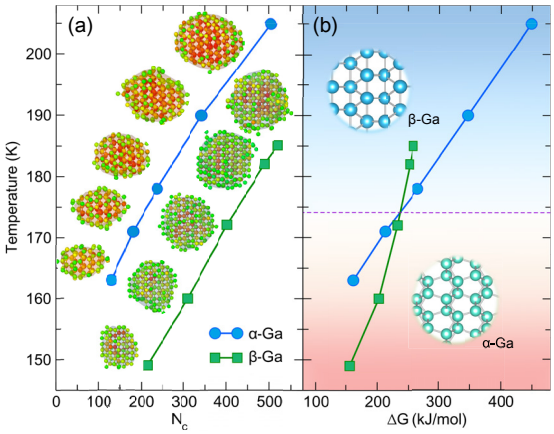

Figure 1: *Nucleation details of two polymorphs of gallium, namely α-Ga and β-Ga. In (a) we report the temperature dependence of the critical nucleus size N_c and in (b) the temperature dependence of the nucleation energy barrier ΔG of α-Ga and β-Ga. The snapshots in (a) depict the critical nuclei at each temperature studied. The dashed line in (b) separates the figure into two zones, above the line β-Ga has a lower nucleation energy barrier than α-Ga and below the line the opposite is true.*

compounds, many of the methods we introduced are of general relevance, and have both been contributed to, and supported, by other MARVEL projects.

a) *Features for atomistic learning* The mapping of a material's structure into features that obey the same symmetry properties of the target of a regression model is one of the key ingredient of successful atomistic machine learning. The fundamental understanding of the nature and properties of these so-called representations has been a core focus of the research of D&D1 groups over the past two years, that has led to the construction of features that are suitable to describe long-range interactions [15] as well as of an efficient N-body iterative contraction of equivariant (NICE) procedure to compute features that are so effective that they can be used together with the simplest, linear regression models [16]. The limitations of some of the most commonly adopted frameworks have also been revealed, namely in terms of pathologic degeneracies implying that there are structurally distinct arrangements of atoms that are mapped onto the same set of features [34]. A quantitative measure of the fitness of a set of features to build a ML model can be obtained by computing the Jacobian of the mapping between atomic displacements and structural features. The principal modes of this matrix measure the sensitivity of the features to atomic displacements, and reveal "normal modes" like patterns that visualize the lo-

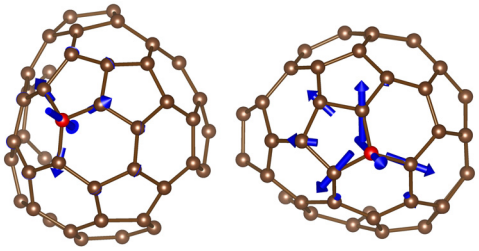

Figure 2: *Two representative eigenvectors for the sensitivity matrix of a SOAP (left) and OM (right) representation of an environment of a defective carbon nanostructure, represented by arrows. The red atom is the central atom.*

calized or collective displacements that couple most strongly to the representation, and then to the properties predicted from the models (Fig. 2). In a collaborative effort that started already in phase 1, and was recently completed, this sensitivity measure was used to compare 5 types of fingerprints that are widely used in machine learning, namely Smooth Atomic Overlap (SOAP), Behler fingerprints (BFP's), modified Behler fingerprints (MBFPs), Faber-Christensen-Huang-Lilienfeld (FCHL) fingerprints and the Overlap Matrix (OM) fingerprints [17].

b) *Molecular and crystal energetics by machine learning* Besides the more fundamental on representations, a major software development effort has been taking place, jointly with the D&D2 and the Inc2 projects, targeting the implementation of an efficient library to compute representations of atomic structures, librascal, and use it to build machine-learning models of the stability of molecular crystals. The code is already available in alpha state [18], and a publication detailing some of the novel performance enhancements which it includes will be submitted in early 2021. Improvements in the accuracy of the underlying energetics could also arise from a ML method to identify deviations of approximate density functionals from exact conditions, that resulted in a model capable of mapping the structure and composition of a molecule to its average energy curvature as a function of the fractional particle number [19]. The availability of an inexpensive uncertainty estimation on the predictions [20] also provides a reliable approach to assess the accuracy of ML models, and to suggest how to improve them in an active-learning fashion [5].

c) *Predicting complex properties by machine learning* Machine-learning models of properties beyond the lattice energy, from NMR chemical shieldings to vibrational spectra, are

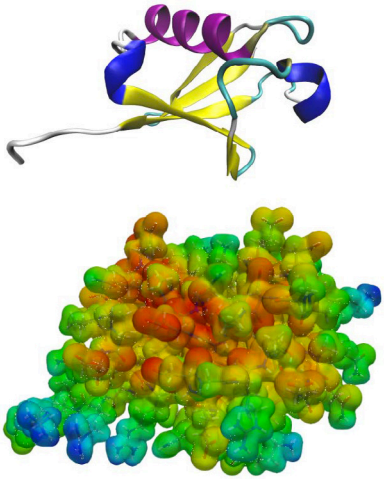

Figure 3: *Top: structure of the ubiquitin protein using ribbon diagram colored according to the different types of secondary structure. Bottom: electrostatic potential map (ESP) of the protein computed from the ML-predicted density. The color code distinguishes the regions with the most negative (red), intermediate (green) and most positive (blue) ESP.*

essential to relate simulations to experimental observables. Thanks to the development of a unique framework to construct machine-learning models of properties that have a tensorial nature [35] we have been able to construct models for several observables that are of high relevance to molecular compounds.

Perhaps the most remarkable advance has been the introduction of a framework to predict the electron charge density, based on learning of the coefficients of an expansion of the density on atom-centered orbitals, using a symmetry-adapted machine-learning algorithm [21]. The first proof-of-principle publication was rapidly followed by more sophisticated models that can predict the charge density of large polypeptides [22, 23] (Fig. 3), and of other density fields such as the on-top density [24]. Symmetry-adapted Gaussian process regression has also made it possible to predict molecular polarizability [25][36] and dipole moments [26], which has been used to estimate the Raman and IR spectra of water [27], and of different polymorphs of molecular compounds [37].

A collaborative effort with the experimental group of Lyndon Emsley (EPFL, chemistry) has focused on the prediction of NMR chemical shieldings, leading to the development of ShiftML [28], a model trained on GIPAW-DFT references of molecular materials, that can be used in tandem with solid-state NMR measurements, to determine the crystal structure of a compound based on small amounts of powder

samples. ShiftML has been used to create an online tool, hosted on the Materials Cloud [29], that predicts in seconds the chemical shieldings for molecular materials containing C, H, N, O, S atoms. In combination with an uncertainty quantification scheme [20], we could develop a Bayesian scheme to match hypothetical crystal structures to solid state NMR experiments [30] — a first example of the convergence of machine learning, modeling and experiments that constitutes one of the grand challenges in this project.

2 Contribution to overall goals and initial proposal

Many of the core goals of the project have been achieved, covering methods to compute the free energies of crystals [3], improvements to structural landscape searches [6], and enhanced sampling to understand nucleation pathways [14]. Despite considerable progress on all these fronts, it has become clear that empirical force fields are not sufficiently accurate to model the subtle energy balance that underlie cohesion in molecular compounds, and that first principles calculations require heroic efforts [1] to even just estimate the relative free-energy of different phases. Machine-learning methods have emerged as the most promising route to address the limitation of present energy and property models, and a large part of the resources in this collaboration have been concentrated on this front, which has led both to fundamental advances in the understanding of the methodology [34][16, 17] and to applications with direct relevance to the behavior of molecular solids. It is also worth mentioning the substantial contributions of this project to the general open data and software efforts within MARVEL: librascal and i-PI have been developed to compute efficiently last-generation ML representations, and to perform advanced sampling calculations. Data from scientific publications has been systematically shared on Materials Cloud, and online tools demonstrating ML models for chemical shifts and molecular polarizabilities have been contributed to the portal [29, 31]. Chemiscope, an interactive structure-property maps visualizer has been released as stand-alone software, and integrated within Materials Cloud [32].

3 Collaborative and interdisciplinary components

This D&D project has been characterized by strong collaborative components, both between its members and in the broader context of MARVEL and outside. We want to highlight in particular four collaborations: (1) that between the Goedecker and von Lilienfeld groups, that resulted in an extensive comparison of representations for machine learning [17]; (2) that between the Corminboeuf and Ceriotti groups, focused on sampling and on the prediction of complex properties of relevance for experiments [5, 21, 22, 23]; (3) that between the Curtin (D&D2) and Ceriotti groups on the development of librascal [18]; (4) that between the Emsley and Ceriotti groups, combining experiments and ML to improve NMR crystallography.

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Design & Discovery 2

From Atoms to Additive Manufacturing: Computational Design of Complex Metal Alloys

Project leader: W. A. Curtin (EPFL, 2MC)

Computational partners: Michele Ceriotti (EPFL, 1MC)

1 Progress

D&D2 has three inter-related thrusts toward the goal of quantitative prediction of metallurgical properties versus microstructure and thermomechanical processing. The first thrust is machine learning (ML) of new interatomic potentials for metals and, especially, alloys. A major part of this thrust is the development of a robust and efficient library for atomic scale learning. The second thrust is the application of the machine-learning potentials to critical issues in metallurgy of selected alloys. The third thrust is making the link between atomistic scale studies, which are always limited in size and/or time scales, to higher-scale methods while maintaining predictive capability. The fourth thrust, stemming from Agility Plus funding at the end of phase 1, is the first-principles-based prediction and design of new high entropy alloys. Here we summarize the major progress in each thrust during phase 2, noting that the project started with phase 2.

1.1 librascal

A major effort in D&D2 has been the development of machine-learning software called librascal. librascal aims to be an efficient, scalable and versatile library for using, comparing, and developing atomic representations for use as a predictor for atomistic/molecular properties including, but not limited to, energies and forces. These representations are the input to any supervised or unsupervised learning algorithm and are often the computational bottleneck. librascal is a stand-alone code written in C++ with flexibility to interface to other established codes like LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) and PLUMED-2.0 (Plugin for Molecular Dynamics) and Python bindings to the core functionality provide ease of use. Computationally-expensive operations are implemented in the C++14 standard with a special focus on efficient data structures and memory-safe design of iteration and data access. The initial emphasis was on implementation of two commonly-used atomistic representations, SOAP and atom-centered symmetry functions (ACSF). Recent emphasis has been on using these representations (and their gradients) for benchmarking and optimizing machine-learning models. The main technical code addition has been a simple, efficient, machine-learning model evaluator for kernel ridge regression (KRR) that encompasses the popular and successful GAP model with SOAP descriptors.

Execution time for one MD step is typically dominated by the energy and force evaluation. This evaluation includes both computing the atomic representation and evaluating the machine-learning model with that representation as its input. In most applications using the SOAP representation and GAP potential, neither the model nor the representation dominates the total time, so both must be optimized in order to achieve a significant reduction in the overall MD runtime. A key optimization for reducing the model runtime is to reduce the size of the computed representation vector. Several selection algorithms are available that can automatically select the most significant components and thereby reduce the dimensionality of the fit space. Reductions up to a factor of 10 are possible without impacting the accuracy of the fit, and this reduction directly translates into a reduction in the computational cost of the model. We have devised a set of benchmarks across several representative systems and covering a wide range of possible model parameters. These benchmarks were run and organized with the signac framework, which also aids in the later curation and data sharing stages. Fig. 1 shows how the computational cost may be reduced by up to a factor of 7 compared to QUIP, the current most popular code used to run SOAP-GAP potentials. These results underscore the importance of the feature dimensionality reduction.

The librascal code is well-poised to become an integral piece of infrastructure in the ML potentials ecosystem for the task of computing

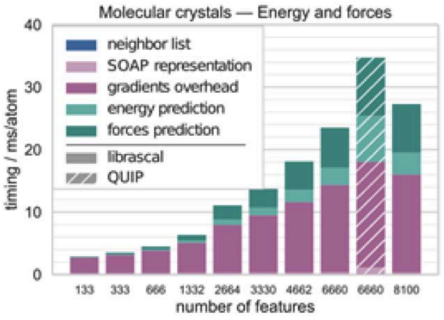

Figure 1: *Effect of the representation (feature) dimensionality reduction optimization on overall prediction runtime, compared to an existing code (QUIP) that does not implement this optimization. In most cases, the number of features can be reduced by a factor of 10 with minimal impact in model accuracy.*

SOAP, symmetry functions, and the many related atomic-scale representations. Its modular design and incorporation of the latest design improvements and optimizations have already led to its adoption in several projects in the COSMO group, including computation of feature vectors for the chemiscope structure-property explorer (with a demo available on Materials Cloud) and as a starting point for recursive evaluation of higher-body-ordered representations. We expect this pattern of adoption to continue as we add capabilities and refine the user interface.

1.2 Machine-learning potentials and applications

We have completed our major efforts on machine-learning potentials for several technologically-relevant lightweight metals and alloys: Al-Mg-Si, Al-Cu, and Mg. While we have been using the Behler-Parrinello atomistic descriptors within a neural-network framework, the overarching goal has been to demonstrate that using an extensive metallurgically-relevant training set for machine-learning yields potentials that can capture a very broad range of metallurgically-relevant properties (dislocations, crack tip behavior, precipitate phases and thermodynamics, early-stage nucleation, etc.). This moves the field away from a focus on *methods* for machine learning, where the training sets are convenient but have typically been insufficient for real metallurgy, to a focus on *applications* that have not been accessible using either first-principles or traditional potentials.

In Al-Mg-Si, our work has culminated in several important results. First, since precipitate shearing controls alloy strength after artificial aging, we have made the first predictions of the generalized stacking fault energy (GSFE) surface for the relevant slip planes (determined here) for three β'' precipitates crucial in the Al-6000 series Al-Mg-Si alloys (Fig. 2) [1]. Post-validation against our new DFT results at selected points shows broad agreement, although the neural net potential (NNP) energies of these very complex faults are slightly (∼15%) higher than DFT. Second, we have performed extensive kinetic Monte Carlo (kMC) studies of the detrimental early-stage natural aging in Al-Mg-Si at room temperature and for commercial compositions. We show the formation of stable multi-solute (Mg, Si) clusters on time scales of minutes, consistent with experimental understanding, but below experimental resolution and never before accurately modeled (Fig. 3). The chemical accuracy of the NNP for these clusters has been post-validated against DFT on selected clusters. We find that these clusters trap vacancies rather strongly, which retards subsequent aging processes, kinetically locking-in a fairly stable natural aging state. These so-called "vacancy prisons" have long been postulated based on a spectrum of indirect data (electrical resistivity, positron an-

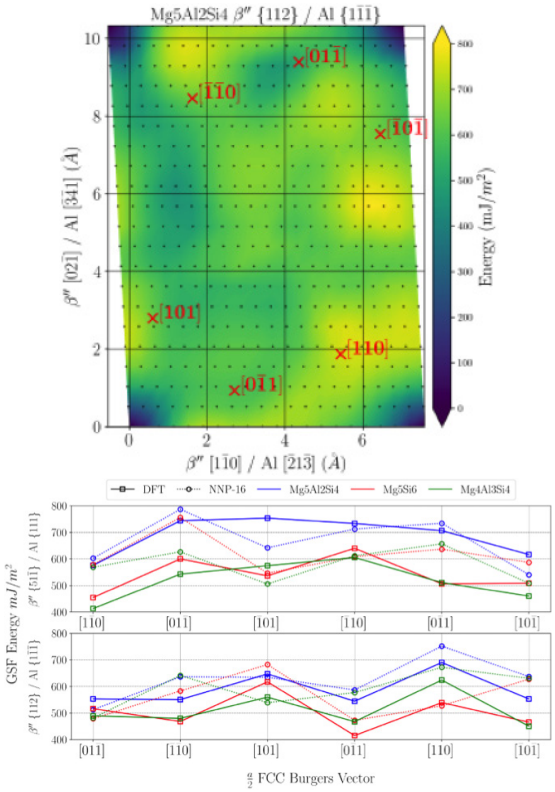

Figure 2: *(a) Generalized stacking fault surface for the 112 slip plane of the $Mg_5Al_2Si_4$ β'' precipitate, with relevant Al Burgers vectors indicated. (b) Fault energies for slip of all possible (110)a/2 type Burgers vectors of Al in the various β'' precipitates.*

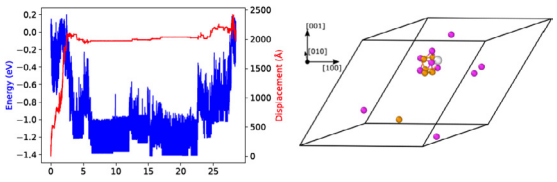

Figure 3: *(a) Evolution of energy and vacancy displacement during early-stage clustering at RT. (b) Typical stable Mg-Si cluster with a trapped vacancy, with total energies computed by NNP and DFT as indicated.*

nihilation, etc.). With this progress, we are in position to pursue the study of new processing strategies (time and temperature) to direct formation of early stage clusters that may be less detrimental, positioning the alloy for enhanced or accelerated artificial aging.

We have completed development of an NNP for binary Al-Cu [2]. This effort was aimed primarly at demonstrating the power of the ML approach for metallurgy in a system that has been very widely studied experimentally and computationally, while having a number of subtle features. Our NNP accurately captures energies for many precipitates, various precipitate GSFEs, and various precipitate anti-site defects, most outside of the training set. The important crossover in thermodynamic stability between θ and θ' precipitates is captured by our new NNP using fully anharmonic analysis (Fig. 4). This Al-Cu potential is being made openly available, and will likely be used by other groups to simulate the evolution of so-called Cu GP zones and θ' precipitates with subsequent molecular statics/dynamics simulations of the strengthening and then simulations of strengthening due to θ' precipitates. To further demonstrate the power of machine learning, we have completed a thorough investigation of the thermodynamics of Ni using an NNP approach [10]. The study includes a wide array of bulk, interfacial, and defect properties from 100 K to 2500 K, and introducing both quantum nuclear fluctuations and electronic entropy when needed.

Because Mg alloys have a high technological importance and because potentials that capture all of the different deformation features in hcp Mg have been lacking, we have also developed a comprehensive NNP for Mg in the Behler-Parrinello framework [3]. We have included many key features for plasticity, such as generalized stacking fault curves for the basal, prismatic, and pyramidal I and II slip systems. The potential captures a range of dislocation core structures in agreement with DFT. The one exception is the pyramidal II screw dislocation,

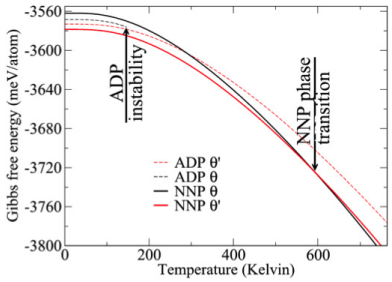

Figure 4: *Helmholtz free energy versus temperature for the θ and θ' precipitates in Al-Cu using the NNP potential, showing a crossover around 600 K; also shown are results for the ADP potential, for which the θ phase is unstable at low T.*

for which the NNP predicts a structure that appears to be a combination of Pyr. I and II screw partial dislocations. The structure and stability of the Pyr. II screw dislocation relative to the Pyr. I screw is crucial understanding how high ductility is achieved in Mg alloys. However, even current DFT studies remain uncertain about the relative stability, and so training a potential based on DFT may lead to an incorrect result. In all other respects, our Mg NNPs are far superior to the best MEAM potential (previously created by our group). We have also improved upon the fracture predictions, relative to the previous MEAM potential, one consequence being that pure Mg is not as brittle as suggested by studies using the standard potential. Most recently, we have tackled the behavior of the prismatic $< a >$ screw dislocation, which is not accessible by DFT [4]. This dislocation is absolutely unstable to dissociation on the basal plane, which is shown by the NNP but not by the MEAM. Prismatic $< a >$ slip thus requires cross-slip of the basal $< a >$ screw onto the prism plane, which is a fully-3D, thermally-activated process. We have been able to study the stress-dependent barrier for this process using the Mg NNP for the first time (Fig. 5). While the barriers are larger than

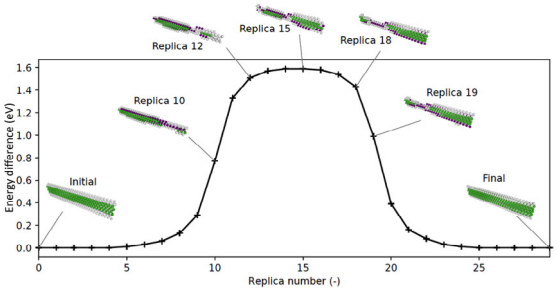

Figure 5: *Transition path and atomistic configurations for $< a >$ slip on the prismatic plane of Mg by basal cross-slip.*

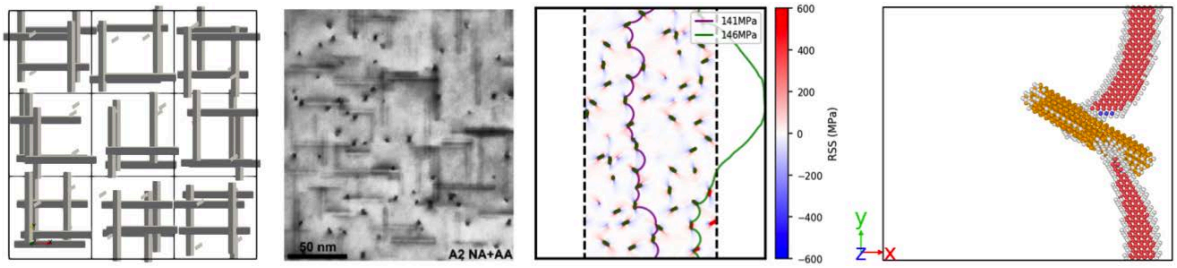

Figure 6: *(a) Realistic pseudo-random microstructure for Al-6xxx at peak aging with corresponding experiment. (b) Critical dislocation line (purple) at the critical point of Orowan looping on a (111) plane in the Al-6xxx microstructure. (c) Fully atomistic simulation, using the new Al-Mg-Si NNP, of a dislocation passing a β″ precipitate.*

experiment, some important trends are consistent, and the deviations point to more-complex mechanisms now under study.

Further work has emerged as a result of our direct D&D2 research. First, we are now working in a team project funded through Materials Design Inc. to develop machine-learning potentials for Zr, Zr-H, and Zr-H-O. We are applying our expertise to ensure that these potentials are broadly applicable to the many metallurgically-critical features of deformation and fracture in hcp Zr. Second, we have collaborated with U. Leoben (Austria) on the understanding of very new Al-Mg-Zn-Cu alloys. These alloys are similar to the Al-Mg 5xxx alloys, at 4-5% Mg, but with added Zn (2-3%) to enable age-hardening (precipitation). It has been discovered experimentally that the addition of just 0.25% Cu leads to faster aging and stronger alloys after aging. Using DFT, we have shown that Cu incorporation into surrogate early-stage η' precipitates is energetically very favorable and we have discovered a new more-stable η' precipitate structure that agrees with available HRTEM data. We have further shown that Cu incorporation (replacing Al or Zn) into the terminal T-phase ($Mg_{32}Zn_{32}Al_{17}$, 162 atom unit cell) precipitate is also energetically very favorable [5]. These results rationalize the experimental findings that the dilute Cu additions lead to faster nucleation of precipitates and a higher final density of precipitates, leading to enhanced strength.

1.3 Higher-scale modeling: Precipitate strengthening in Al-Mg-Si

In parallel with our atomistic studies, we have completed a higher-level continuum discrete-dislocation modeling of the strength of the peak-aged alloy [6]. We have created a series of realistic β'' precipate morphologies based on experimental observations and have simulated the motion of screw and edge dislocations through the alloy microstructure (Fig. 6). Many features of this modeling go beyond the state of the art. Results show that the stress for Orowan looping around the precipitates is typically 44% larger than experiments, indicating that strength is controlled by precipitate shearing (although textbook analysis suggests that these processes should have equal strength at peak aging). We have thus pursued precipitate shearing theoretically using our DFT-computed GSFEs for β'' shearing (see above). Estimated alloy strength is then approaching the experimental values. Finally, as a first application of the NNP in a direct simulation of dislocation/precipitate interactions, we are observing the shearing process and role of misfit stresses directly, and are close to making contact with experimental scales and continuum simulations. These last results demonstrating the high combined value of quantitative, broadly-applicable machine-learning potentials plus larger-scale studies to reach experimental scales and microstructural complexity.

1.4 High entropy alloys

High entropy alloys (HEAs) are separate from the precipitation-strengthened alloys of main interest in D&D2 but represent a major opportunity for additive manufacturing (AM) because HEA are random alloys with properties that are expected to be robust against the severe processing conditions typical of AM. HEAs will be a major focus of a phase 3 proposal in the metallurgy domain. With significant initial successes, we have pursued further studies, applications, predictions, and extensions of our combined theory and computational approach. We have consistently achieved quantitative success in predictions of the yield stress at experimental conditions (imposed temperature and strain rate).

Our baseline theory requires the computation of solute misfit volumes, alloy elastic

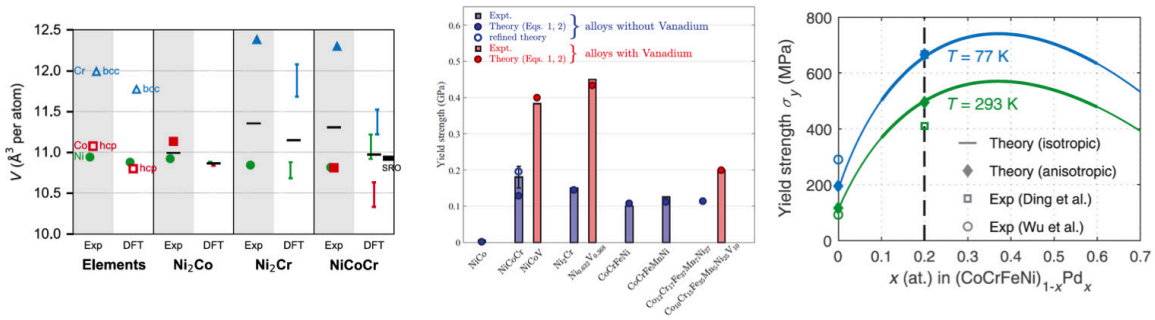

Figure 7: *(a) Volume per atom in various Ni-Co-Cr alloys, as measured and as predicted by spin-polarized DFT, showing the very poor DFT predictions for NiCoCr due to Co-Cr magnetic interactions. (b) Yield strength versus alloy, for a range of fcc alloys; the addition of Vanadium increases the strength in all alloys. Experiments: bars; Theory: symbols. (c) Yield strength versus Pd content in random CoCrFeNi-Pd alloys, at low and room temperature, with experiments also shown.*

constants, and occasionally alloy stable stacking fault energies. We have now successfully understood/predicted the strength of NiCoCr [7]. We have also shown that, unfortunately, DFT computations of the misfit volumes in this alloy are poisoned by Co-Cr magnetic interactions and hence are inaccurate (compared to experiments performed at our direction by collaborators in Japan) (Fig. 7a). We have also investigated NiCoV, which is measured to be nearly 2× as strong as NiCoCr. Here, magnetism presents no problem, and the large misfit of V is the source of the high strength. Quantitative agreement with experiments is obtained on both NiCoV and $Ni_{63.2}Co_{36.8}$. We have also shown that the new alloy $Co_{10}Cr_{15}Fe_{35}Mn_5Ni_{25}V_{10}$ has high strength due again to V [8]. In general, we predict that V is an excellent element for strengthening in both fcc and bcc HEAs, relative to other elements in these families, and this prediction is broadly observed experimentally across many different alloys (Fig. 7b). Finally, recent work published in *Nature* suggested that CoCrFeNiPd was much stronger than CoCrFeNi due to a nanoscale segregation of Pd-rich and Ni/Co-rich domains. We predict that, due to the large misfit of Pd in CoCrFeNi, that the strength of random CoCrFeNiPd is essentially equal to the measured strength (Fig. 7c) [9], so that the nanoscale segregation is not necessary to achieve high strength.

Our newest theory includes direct solute-solute interactions in the random alloy. We have thus pursued DFT computation of these solute-solute energies. Specifically, for a family of noble metal alloys (Au-Ag-Cu-Pd-Pt-Ni) and using SQS supercells, we compute total energies for many different realizations of a given alloy family around a target composition and decompose the total energy into effective pair interactions (EPIs) versus pair distance with high accuracy. We are using these EPIs in our new theory to refine strength predictions for random alloys. Results for AuNiPdPt show a large difference between theory and recent experiments, from which we have deduced that this alloy is not random. To demonstrate this, Monte Carlo simulations using our EPIs reveal nanoscale segregation in AuNiPdPt even just below melting. The trends are, furthermore, very consistent with new (unpublished) atom probe tomography experiments by German collaborators. Thus, when our theories fail, we are able to deduce that there is additional physics, in this case ordering phenomena, which is then both predicted and confirmed experimentally.

2 Collaborative and interdisciplinary components

This project is a collaboration between LAMMM (Curtin), providing the main expertise in metallurgy and mechanical properties, and COSMO (Ceriotti), providing the main expertise in advanced machine-learning methods and thermodynamics. The librascal development is an intimate collaboration involving many members from both labs. The Al-Mg-Si work has been done with a shared LAMMM-COSMO post-doc (Glensk) with LAMMM post-doc Jain interacting regularly with Ceriotti on kMC simulations and analysis of precipitation, and LAMMM PhD student Marchand working closely with the AiiDA team. COSMO is now using the new HEA data on noble metal alloys from LAMMM as a baseline for machine learning in complex alloys.

MARVEL publications

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

[1] A. Jain, D. Marchand, A. Glensk, M. Ceriotti, and W. Curtin, *in preparation* (2021).

[2] D. Marchand, A. Jain, A. Glensk, and W. A. Curtin, *Machine learning for metallurgy I. A neural-network potential for Al-Cu*, Physical Review Materials **4**, 103601 (2020).

[3] M. Stricker, B. Yin, E. Mak, and W. A. Curtin, *Machine learning for metallurgy II. A neural-network potential for magnesium*, Physical Review Materials **4**, 103602 (2020).

[4] M. Stricker and W. A. Curtin, *Prismatic Slip in Magnesium*, The Journal of Physical Chemistry C **124**, 27230 (2020).

[5] L. Stemper, M. A. Tunes, P. Dumitraschkewitz, F. Mendez-Martin, R. Tosone, D. Marchand, W. A. Curtin, P. J. Uggowitzer, and S. Pogatscher, *Giant hardening response in AlMgZn(Cu) alloys*, *submitted* (2020).

[6] Y. Hu and W. A. Curtin, *Modeling peak-aged precipitate strengthening in Al-Mg-Si alloys*, *submitted* (2020).

[7] B. Yin, S. Yoshida, N. Tsuji, and W. A. Curtin, *Yield strength and misfit volumes of NiCoCr and implications for short-range-order*, Nature Communications **11**, 2507 (2020).

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[9] B. Yin and W. A. Curtin, *Origin of high strength in the CoCrFeNiPd high-entropy alloy*, Materials Research Letters **8**, 209 (2020).

Other references

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Design & Discovery 3

MARLON: MARVEL Design, Discovery and Engineering of Low-Dimensional Materials and Nanostructures

Project leader: Nicola Marzari (EPFL, 1.5MC)

Computational partners: Mathieu Luisier (ETHZ, 1.2MC), **Daniele Passerone** (Empa, 1MC), **Alfredo Pasquarello** (EPFL, 0.5MC), Clémence Corminboeuf (EPFL)
Experimental partners: Kumar Agrawal (EPFL), Oliver Gröning (Empa), **Roman Fasel** (Empa, 0.5MC)

1 Progress of the different efforts

D&D3 is dedicated to the design or discovery of novel low-dimensional materials and nanostructures, and in the engineering and integration of these into novel architectures, devices, and processes.

1.1 Novel low-dimensional materials

This subproject builds on and expands the results obtained in our first high-throughput [1] screening effort, where starting from the 3D structures of two experimental databases (ICSD and COD) we identified 1825 inorganic materials that could be exfoliated into novel monolayers. Thanks to the inclusion of a third database (Pauling File), updated version of COD and ICSD and refinements in the screening procedure, we expanded our search finding other 1252 new materials, for a total portfolio of more than 3000 different inorganic materials that can be exfoliated in monolayers. Remarkably, more than 800 of these new materials exhibit a binding energy similar to other monolayers already isolated experimentally, suggesting the possibility of straightforward exfoliation. For the entire expanded database of 2D materials we have now run an extensive characterization of fundamental properties including band structures, band alignments, density of states, effective masses, phonons at the Γ-point and static dielectric tensors. On a subset of 1282 materials (those with less than 12 atoms per unit cell) we also performed calculations of the full phonon dispersion as well as the determination of the magnetic ground state.
In a parallel effort we built a new database focused on 1D materials that could be potentially isolated from weakly bonded 3D parents. Both experimentally and theoretically the study of novel 1D structures is still in his infancy. Some experimental studies on quasi-1D materials, however, already showed the great potential of these compounds as conductors, photodetectors and photocatalysts. Using a computational procedure similar to the one adopted for the 2D materials we identified 815 unique 1D wires and computed their binding energy as a measure of the possibility to isolate a single wire. Furthermore, we built a database of properties ranging from electronic band structure and alignment to phonon dispersion relations that will allow the efficient pre-selection of materials for application-oriented targeted studies and that are already revealing part of the interesting typical of 1D systems especially in relation with charge density instabilities.

a) *Photocatalytic water splitting* Hydrogen production through photocatalytic water splitting represents a promising approach for solar power conversion and the identification of new potential photocatalysts is crucial to empower its sustainable large scale application. Initially starting from the 2D structures database created in year 4 [1], and its subsequent characterization, we selected 147 promising candidates for solar-driven overall water splitting; of these, 48 have been excluded on the basis of their stability or composition, 31 were known, validating our approach while 68 were previously unreported greatly expanding the number of predicted photocatalysts. Each one of the 99 materials suitable for applications has been studied in greater detail with the inclusion of the optical absorption spectra, estimates of the excitonic binding energy as well as the stability in aqueous environments. This process allowed us to capture a very wide picture (summarized in Fig. 1) on how the 2D materials considered can perform in photocatalytic water splitting on the basis of multiple descriptors. More recently the screening has been expanded to the most up-to-date version of the 2D database, as well as ad-hoc engineered heterostructures.

b) *2D BCS superconductors* Superconductivity in 2D materials is a rare property, few materials exhibit conventional BCS superconduc-

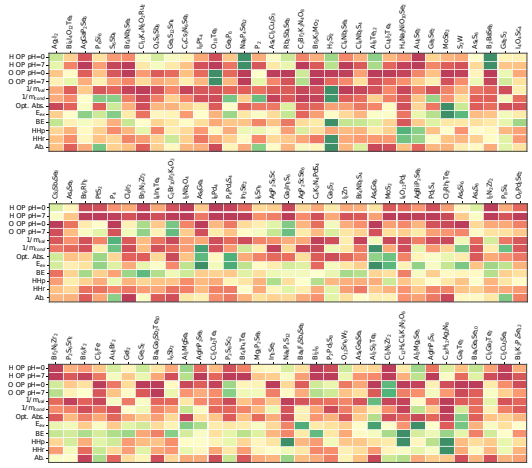

Figure 1: *Summary of the relevant properties for the 99 non-toxic and dynamically stable materials identified in this screening.*

tivity down to the single monolayer and generally the transition temperatures hardly exceeds 5 K. To find new and possibly better candidates for 2D superconductors, we explored almost 100 materials, computing the transition temperature from a brute force integration on the Brillouin zone of the electron-phonon coupling elements. To cope with the computational cost and the difficulties in the integration of tiny disconnected part of the Brillouin zone we restricted our screening to 2D metals with less than 6 atoms per unit cell. Even so, we found 12 materials with a computed transition temperature higher than 5 K with the most noticeable case reaching almost 20 K. More accurate estimates obtained from the full solution of Migdal-Eliashberg equations (Fig. 2) place the transition temperature above the 21 K mark of liquid hydrogen; moreover, we have shown that the electron-phonon coupling and consequently the transition temperature can be strongly tuned with both doping and strain. Interestingly the material is predicted to have a non-trivial band topology with chiral edge states above the Fermi level that could possibly be reached in heavy electron-doping conditions opening the possibility for exotic interactions with the superconducting phase.

1.2 Novel two-dimensional devices

Here, we focus on the modeling of the device characteristics of 2D materials, by combining density-functional theory and quantum transport calculations, and integrating those with the materials database of the first subproject. A dedicated framework has been developed that was awarded the ACM Gordon Bell Prize in High Performance Computing in 2019 [2].

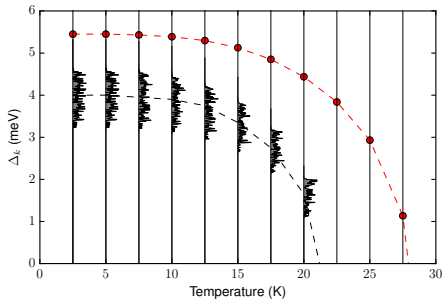

Figure 2: *Evolution of the superconducting gap as a function of temperature computed by solving the Migdal-Eliashberg equations in the isotropic approximation (red dots) and with a fully anisotropic solution where the grey histograms show the magnitude distribution of the momentum-dependent superconducting gap.*

a) *Ultra-scaled transistors* Starting from the database [1], the "current vs voltage" characteristics of single-gate, ultra-scaled field-effect transistors (FETs) made of 100 different 2D monolayers, as shown in Fig. 3, have been computed. Thirteen promising candidates with a ballistic ON-state current larger than 3000 μA/μm, both in their n- and p-type configurations, have been identified, among them known (GeS, GeSe, black phosphorus) and novel (Ag_2N_6 or O_6Sb_4) 2D materials [3]. In terms of current, they outperform most conventional transition metal dichalcogenides (TMDs) by a factor of 3, except WS_2, which reaches an almost comparable performance. From these investigations, a database was created that covers the band gap, effective mass, dielectric constant, $I-V$ characteristics, gate

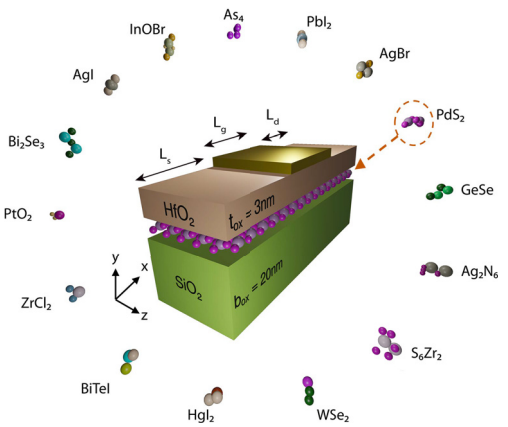

Figure 3: *Schematic view of the single-gate field-effect transistor structure that served as benchmark to compare 100 different 2D channel materials. The latter (here PdS_2) are placed on a SiO_2 box and separated from the gate contact by a HfO_2 oxide layer. The primitive unit cells of few representative 2D materials are plotted around the transistor structure.*

length scalability, injection velocity, and inversion charge of all compounds. To refine the analysis of the best performing 2D materials, their mobility is currently being calculated in collaboration with EPFL, including not only electron-phonon interactions, but also charged impurity scattering [4]. Furthermore, we have started examining metals forming low contact resistances with selected 2D monolayers using the approach of [5].

b) *Thermal properties of van der Waals materials* Two-dimensional monolayers, when stacked on top of each other in van der Waals materials (vdWms), possess peculiar thermal properties that have been simulated with our *ab initio* quantum transport solver. By combining various MoX_2 and WX_2 TMDs with each other, as illustrated in Fig. 4, it has been found that homogeneous vdWms made of the same top and bottom 2D materials "simply" scale the thermal current that flows through them, while heterogeneous vdWms (the two 2D materials are different) act as low-pass filters for phonons [6]: only the acoustic branches are smoothly transferred from one monolayer to the other. These results could have implication in the design of nanoscale thermo-generators, where low thermal conductivities are needed.

c) *Majorana transport in 2D materials* Several 2D materials exhibit high spin-orbit coupling energies, a feature that is key to enable Majorana fermions and the creation of topological qubits for quantum computing systems. The simulation framework that has been put together to model 2D FETs has been extended to support Majorana transport, which requires to account for the so-called proximity effect of a superconductor and the influence of magnetic fields. This was achieved by applying Bogoliubov-de Gennes (BdG) transformation. Two 2D materials have been investigated, a conventional (WSe_2) and a novel (PbI_2) one. In both cases, a Majorana zero mode (MZM) could be detected in bandstructure-only calculations. The presence of a MZM has been further confirmed in device simulations from first-principles using up to 140'000 atoms. The outcome has been presented at the International Electron Device Meeting (IEDM) 2020.

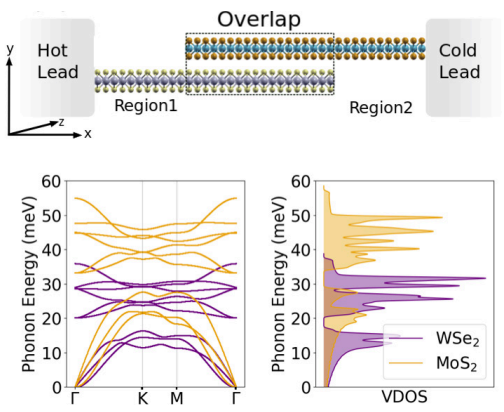

Figure 4: *(top) Artistic representation of a van der Waals material composed of two 2D monolayers stacked on top of each other with a partial overlap in the middle and different electrode temperatures. (bottom) Phonon bandstructure and density-of-states of MoS_2 (orange) and WSe_2 (magenta).*

1.3 Novel low-dimensional nanostructures

Here, we explore the potentiality of graphene nanoribbons (GNRs) in ultra-scaled transistors. Earlier work based on *ab initio* simulations has shown that their performance is principally limited by their high contact resistance. Starting from the prototype realized at Empa, we demonstrated an improved GNR FET that overcomes the contact limitations. The key improvements were (i) the definition of an optimal GNR-lead relative orientation and (ii) the inclusion of metal adatoms as electronic bridge between the contact and channel. GNRs are now synthesized on Au(111) terraces that yield batches of aligned GNRs [7].

a) *Optimization of contacts* Simulations have also moved to the exploration of GNR FETs with metallic side contacts. Results show that the in-plane hybridization between the metal and carbon atoms can significantly improve the injection efficiency of charge carriers into the GNRs. We employ a machine learning scheme in conjunction with a recently developed method to extract a set of localized orbitals [8] to refine the analysis of the best performing prototypes. We consider a selection of material and surface orientation for the contacts. A reduced resistance is reported for metals with outermost shell electrons in *d*-type orbitals. In the vicinity of the surface, the GNRs "benefit" from the degrees of freedom from the surface metal atoms, resulting in efficient transfer of electrons.

b) *"Smart" basis sets* In collaboration with TU Wien, we are developing an unprecedented computational tool based on non-equilibrium Green's function (NEGF) and dynamical mean-field theory (DMFT) for calculating the conductance in correlated regimes. The simulation framework has been put together [8] with the development of a new basis set to support correlation in transport in a "lightweight" approach. This is achieved by deterministic ex-

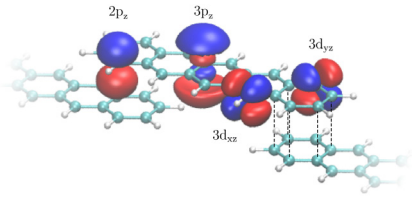

Figure 5: *Schematic visualization of the subset of relevant LOs identified from the process of subdiagonalization for the polyacene junction.*

trapolation from the *ab initio* calculation of a minimal basis set that correctly describes the physics around the Fermi energy. For organic structures a single local orbital (LO) per atom (Fig. 5) is sufficient, thus making this basis naturally suited for DMFT. We have started examining 5-AGNRs which display the most pronounced Coulomb blockade diamonds.

c) *Magnetic nanostructures* In parallel to the activity focused on real devices, the search for novel carbon based nanostructures has moved towards materials expressing magnetic properties. To induce magnetic properties in nanographenes we followed successfully several different routes: topological frustration [9], sublattice unbalance [10], design of topologically protected states [11] and design of heterostructures containing porphyrines [12, 13]. The results obtained for triangulene dimers [10], for coupled spin states in armchair nanoribbons [11] and for porphyrin containing GNRs [13] (Fig. 6) have particular relevance and open a new research effort toward the fabrication and characterization of 1D spin chains. Of relevance also the fabrication of a device based on a GNR with massive Dirac fermion behavior [14]. Research in this field was considerably boosted thanks to the enrollment of experimentalists in the execution and analysis of part of the simulations needed. This was possible thanks to the latest developments in AiiDAlab.

1.4 Low-dimensional catalysts

A bifunctional oxygen evolution reaction (OER) mechanism has recently been proposed as a possible explanation for the low overpotentials observed in the case of a novel NiOOH/FeOOH catalyst [15][18]. In this mechanism, a second, functionally different active site acts as hydrogen acceptor. Thus, the limitations imposed by the linear scaling relationship between the intermediates of the conventional OER mechanism are avoided. First, we investigated the conditions under which the bifunctional mechanism outperforms the

Figure 6: *Pictorial representation of the experimental approach to the production of porphyrine containing graphene nanoribbons at Empa.*

regular OER mechanism. We chose a selection of potential catalysts and considered all potential pairings in order to establish the properties conducive to low overpotentials within the bifunctional scheme [16]. We have found that under anodic conditions, the hydrogen binding energy, which plays a critical role in the thermodynamic description of the bifunctional mechanism, is correlated with the valence band maximum of the catalyst acting as hydrogen acceptor. Moreover, this preliminary study identified pairings of materials that exhibit OER overpotentials as low as 0.27 V, demonstrating the ability of the bifunctional mechanism in overcoming the limitations associated with the linear scaling relationships Then, a detailed study of the NiOOH and FeOOH catalysts was carried out. We focused on the detailed interface between the two materials as described experimentally in the work by Song *et al.* [15]. We have investigated several possible models for both the FeOOH nanoparticles, which act as the main catalyst, as well as for the NiOOH substrate, which acts as the hydrogen acceptor [17]. The best performing pairings of these models were interfaced in a single computational cell and the performance of each bifunctional catalyst was obtained. An explicit interface that exhibits many of the experimentally identified structural features showed an overpotential of just 0.26 V, which is in good agreement with the result reported for this bifunctional catalyst [15][18].

2 Contribution to overall goals and initial proposal

D&D3 is very closely aligned to the overall goals of the MARVEL project: to discover

novel materials, to ramp up simulations to be able to investigate entire devices, and to do this in close collaboration with experimentalists, in addition to developing novel methods. EPFL, ETHZ and Empa are doing this by joining forces to shed light on the performance of next-generation transistors based either on novel 2D materials or graphene nanoribbons and to explore novel applications that bear a lot of potential, from superconductors to photocatalysts to thermo-generators and quantum computing systems. Several tools must be combined with each other to investigate such structures from the atom to the device level, and these are all code cores for MARVEL: QUANTUM ESPRESSO, CP2K, Wannier90, and OMEN.

3 Collaborative and interdisciplinary components

Apart from their mutual interactions, EPFL, ETHZ, and Empa also collaborates with researchers outside of MARVEL, e.g. Lukas Novotny (ETHZ), Andrea Ferrari (U. Cambridge), Francesco Mauri (La Sapienza), Eric Pop (Stanford), Aaron Franklin (Duke University), and Adrian Ionescu (EPFL). All fabricate devices based on 2D materials and are eager to benefit from computer-assisted design guidelines. We also work closely with Torsten Hoefler (ETHZ) on the improvement of the computational performance of OMEN and with Nicolas Cavassilas (University Aix-Marseille) on the realization of a water-splitting system relying on heterojunctions of 2D materials.

MARVEL publications

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

- [1] N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi, and N. Marzari, *Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds*, Nature Nanotechnology **13**, 246 (2018).
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- [3] C. Klinkert, Á. Szabó, C. Stieger, D. Campi, N. Marzari, and M. Luisier, *2-D materials for Ultra-scaled Field-Effect Transistors: One Hundred Candidates under the Ab Initio Microscope*, ACS Nano **14**, 8605 (2020).
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Design & Discovery 4 Nanoporous Materials Genome: Optical, Catalytic and Electronic Properties

Project leader: Berend Smit (EPFL, 2.33MC)

Computational partners: Jürg Hutter (UZH, 1.5MC), **Alfredo Pasquarello** (EPFL, 1.5MC), **Ivano Tavernelli** (IBM, 1MC)
Experimental partners: Marco Ranocchiari (PSI, 0.33MC + 0.33MC from PSI), **Emiliana Fabbri** (PSI, Agility Plus, 0.4MC + 0.4MC from PSI)

1 Progress of the different efforts

D&D4 aims to develop and apply computational method to better understand the properties of metal organic frameworks (MOFs). An important aim for phase 2 in MARVEL is to demonstrate that computational materials design can result in novel materials. In D&D4 we have now three examples in which we computationally design a novel material that was subsequently synthesized. These examples are related to fundamental questions on how to tune the optical and electronic properties of MOFs. A major breakthrough was achieved to design novel materials for carbon capture. A key challenge was to find a material that can capture CO_2 in wet flue gasses. The material that was discovered computationally and subsequently synthesized in D&D4 outperformed commercial materials.

Another important aim in D&D4 has been the development of efficient computational techniques to determine the optical and electronic properties of MOFs. Significant progress has been made to efficiently compute band gaps and the lifetime of electron-holes.

The experimental work in D&D4 has focussed on using the unique properties of MOFs to carry out catalysis that has not been possible using the conventional catalysts.

As Open Science project, a workflow has been developed in D&D4 to maintain a library of curated experimental covalent organic frameworks (COFs). This library has grown from 300 to over 600 structures and is fully implemented using the AiiDA infrastructure.

The development of novel computational technics have focussed on optical and electronic properties of MOFs, while the application focussed on gas separations (e.g. CO_2 capture from flue gasses) and gas storage (e.g. hydrogen and natural gas). The experimental work has focussed on the exploration of gas separations, (photo-)catalysis, sensing, and other applications of MOFs.

2 Contribution to overall goals and initial proposal

a) *Materials Design* One of the main aims of phase 2 of MARVEL is to apply computational methods to design novel materials. The following materials have been computationally designed and subsequently synthesized.

Tuning the optical adsorption spectrum of MOFs For photocatalysis it is important to tune the optical adsorption spectrum. Using DFT calculations, Anderson *et al.* [1] showed that by changing the lanthanide in Ln-SION-1, one can tune the optical absorption from the UV region to absorption that includes a large part of the visible region. These predictions were subsequently experimentally confirmed.

Metal doping of MOFs Partial metal replacement, or metal doping (Fig. 1), within secondary building units is a promising, yet relatively unexplored route to modulate these properties in MOFs. Syzgantseva *et al.* [2] used DFT calculations to predict effect of doping by Ni on the color of the material. Subsequent synthesis of the doped material confirmed the color change.

Capturing CO_2 in wet flue gasses Boyd *et al.* [3] carried out a large-scale screening study to identify MOFs that can capture CO_2 in the presence of water. Several materials were identified and the subsequent synthesis and testing of these materials confirmed that, even in wet flue gasses, the materials could capture CO_2. In addition, testing in a separation device showed that these materials outperform the conventional materials.

b) *Method developments* One of the main strengths of MARVEL is the development of novel computational methods. Within D&D4, the following methods have been developed in phase 2.

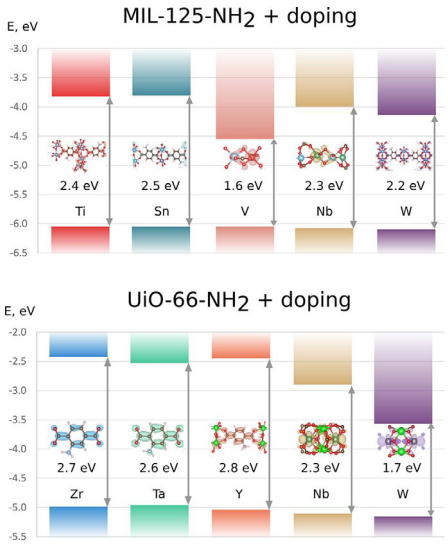

Figure 1: *Band alignment in doped MIL-125-NH_2 and UiO-66-NH_2. Ti and Zr correspond to undoped compounds (from [2]).*

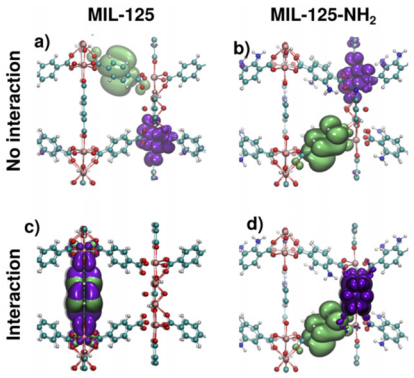

Figure 2: *Isodensity representation of the photo-excited electron (violet) and hole (green) in MIL-125 and MIL-125-NH2. (a,b) Non-interacting charge carriers calculated separately. (c,d) Interacting charge carriers: triplet calculations (from [5]).*

Descriptors for photocatalytically active MOFs Fumanal *et al.* [4] developed a systematic computational protocol to determine two energy-based descriptors that are directly related to the performance of a MOF as a photocatalyst. These descriptors assess the UV-vis light absorption capability and the band energy alignment with respect to redox processes and/or co-catalyst energy levels. This method allows the high-throughput screening of new promising photoactive systems.

Accurate band gaps of MOFs at a lower computational cost In the group of Pasquarello state-of-the-art GW calculations have been performed for a set of MOFs to establish benchmark values for their fundamental band gaps. For the case of MIL-53(Fe), we demonstrated that spectra calculated through the solution of the Bethe-Salpeter equation are in good agreement with optical absorption spectra. Next, it was investigated how to achieve accurate band gaps of MOFs at a lower computational cost. For this, we employed advanced electronic structure calculations based on non-empirical hybrid functionals and focused on a selection of nine MOFs. This study showed that non-empirical hybrid functionals can provide a reasonable accuracy at a significantly lower computational cost than GW calculations.

Defect energy levels involving ionic polarization Interest in optical transitions involving defect states has been growing in recent years for their potential in optoelectronic and photovoltaic applications. In the context of MOFs, defects, such as polarons, affect the luminescence lifetimes (Fig. 2) and the catalytic performances [5]. In order to calculate accurate vertical transition energies via density functional theory, the spurious finite-size effects related to the long-range nature of the electric field associated to the defect need to be accounted for. Such effects can be addressed by applying a posteriori correction schemes. In this regard, we developed a scheme for finite-size corrections of vertical transition energies and single-particle energy levels involving defect states with built-in ionic polarization in the context of supercell calculations. The method accounts on an equal footing for the screening of the electrons and of the ionic polarization charge arising from the lattice distortions. This allows for identifying defect signatures in measured optical spectra without requiring computationally prohibitive system-size scalings. This work has been published in *Physical Review B, Rapid Communication* [6].

Methods to compute near-edge X-ray absorption spectroscopy (XAS) In the group of Hutter a novel method for the simulation of near-edge X-ray absorption spectroscopy (XAS) has been implemented in the CP2K software package. The linear-response time-dependent density functional theory (LR-TDDFT) based method exploits the localized nature of core electronic states and Gaussian basis sets, allowing for efficient calculations of large and periodic systems. The cost of such calculations exhibits a favorable sub-cubic scaling for sparse systems and can be significantly reduced by exploiting GPUs. To match measurements, the simulated spectra need to be rigidly shifted, either empirically or based on some other *ab initio* calculation. To tackle this issue, a new GW based correction scheme was implemented. It

exploits the same efficient approximations as the main LR-TDDFT method and can therefore be seamlessly integrated into the simulation workflows, yielding corrected XAS LR-TDDFT spectra from single calculations.

Wavefunction based correlation methods MP2, RPA, double-hybrids are computationally very demanding for condensed phase systems. Kuehne *et al.* [7] have further improved the implementation in CP2K using numerical advancements, new resolution of the identity methods, and range-separated correlation methods to reduce basis set dependence. The new implementations result in speedups of up to an order of magnitude and have been tested on molecular crystals [8].

c) *Supporting experimental work* The experimental work in D&D4 focusses on (photo-)catalysis. This year, Emiliana Fabbri (PSI) has joined MARVEL through an Agility Plus grant. Her research focussed on the development of MOF-based catalysts to serve as anodic electrodes for the electrochemical splitting of water. Interesting experimental results include the following developments.

Co-catalysed hydroformylation of olefins Bauer *et al.* [9] discovered that the micropores in MOFs push homogeneous catalytic reactions into kinetic regimes inaccessible under standard conditions. Such property allows branched selectivity up to 90% in the Co-catalysed hydroformylation of olefins without directing groups, not achievable with existing catalysts. This finding has a big potential in the production of aldehydes for the fine chemical industry. Monte Carlo and density functional theory simulations combined with kinetic models show that the micropores of MOFs with UMCM-1 and MOF-74 topologies increase the olefins density beyond neat conditions while partially preventing the adsorption of syngas leading to high branched selectivity. This effect, which we call adsorption-driven kinetic modulation (AKM) has important consequences in catalysis.

Detecting fluor in water Ebrahim *et al.* [10] developed a novel lanthanide-based luminescent metal-organic framework, named SION-105 (Fig. 3), with a boron (B) receptor site whose interactions with F^- in aqueous solutions are simultaneously electrostatic and specific in nature because of its carefully designed structural environment. SION-105 has been combined with a portable prototype sampling device that was designed and built in-house to measure F^- concentrations in natural groundwater samples taken from three different countries, with the results showing excellent agreement with ion chromatography analysis.

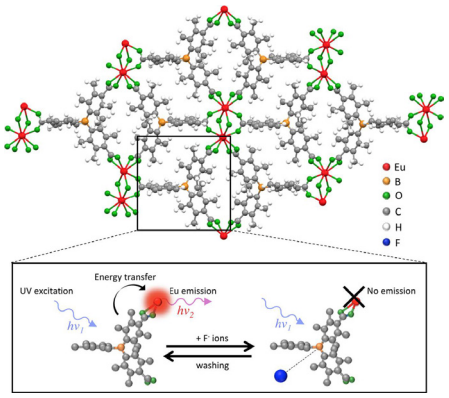

Figure 3: *Structure of SION-105 and (below) its turn-off optical sensing mechanism, whereby the interaction of F^- ions with the Lewis acid B binding site of the ligand leads to quenching of the Eu^{III} emission. H atoms are omitted for clarity (from [10]).*

d) *Open Science* Within D&D4 the following Open Science activities are highlighted.

Curated COFs Ongari and co-workers [11, 12] developed a workflow (Fig. 4) to maintain a database of experimental COFs reported in the literature. The full workflow has been encoded in AiiDA. Both the workflow and the automatically generated provenance graph of the calculations are made available on the Materials Cloud, allowing peers to inspect every input parameter and result along the workflow, download structures and files at intermediate stages, and start their research right from where this work has left off. In particular, our set of CURATED (Clean, Uniform, and Refined with Automatic Tracking from Experimental Database) COFs, having optimized geometry and high-quality DFT-derived point charges, are available for further investigations of gas adsorption properties.

3 Collaborative and interdisciplinary components

Within D&D4 the collaborations focus on method development, open science, and collaborations with the experimental groups. For example the development of novel methodologies to compute the optical and electronic properties of MOFs is the result of collaborations between the groups of Travernelli and Smit [4, 13, 14, 15, 16], and Pasquarello and Smit [5]. Many of these calculations are using the CP2K code that is developed in the

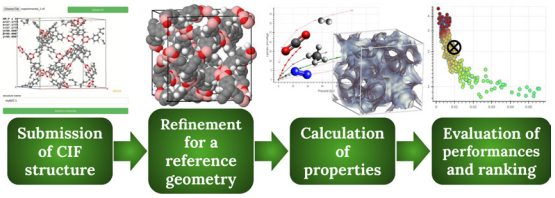

Figure 4: *Scheme of exemplary workflow. The user starts by uploading the atomic structure of a crystalline materials in the CIF format, which triggers the refinement of the atomic positions, the computation of pore geometry, and thermodynamic and transport properties. Finally, its performance for specific applications is evaluated, and the material is ranked versus other candidates (from [12]).*

group of Hutter. The experimental collaborations include the group of Pasquarello and Stylianou [17] and Ranocchiari and Smit [9]. The Open Science projects include the collaboration of the Marzari and Smit groups related to the Materials Cloud [18] and AiiDAlab [19].

MARVEL publications

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

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Design & Discovery 5 Correlated Transition Metal Oxides and Heterostructures

Project leader: Nicola Spaldin (ETHZ)

Computational partners: Ulrich Aschauer (UniBE, 1.25MC), **Claude Ederer** (ETHZ, 1.25MC), **Philipp Werner** (UniFR, 1.5MC)
Experimental partners: Marisa Medarde (PSI), **Urs Staub** (PSI, 0.65MC + 0.65MC from PSI), **Marta Gibert** (UZH, Agility Plus, 0.8MC)

1 Progress of the different efforts

1.1 Correlated oxides

Building on our work during phase 1, the team at ETHZ demonstrated how the coupling between the metal-insulator transition (MIT) and the structural breathing mode distortion in rare earth nickelates gives rise to a first order coupled phase transition. Thereby, the presence of a spontaneous electronic instability towards charge disproportionation is crucial to stabilize the structural distortion [1]. Furthermore, our charge self-consistent DFT+DMFT calculations, using interaction parameters obtained within the constrained random phase approximation (cRPA), allow to obtain equilibrium amplitudes of the structural distortion across the series which are in excellent agreement with experimental data [2]. Our calculations also indicate, in agreement with other work [18], that the coupling to the magnetic order is crucial to stabilize the structural distortion for both $NdNiO_3$ and $PrNiO_3$, i.e., for the systems with the largest rare earth cations in the series. Employing two instructive case studies for orbitally polarized $CaVO_3$ and site-polarized $LuNiO_3$, we also analyzed the effect of charge self-consistency in DFT+DMFT calculations, thereby highlighting in particular the role of the so-called double counting correction [3].

The UniFR group has continued to improve and extend the equilibrium GW+DMFT framework developed in MARVEL phase 1, and systematically tested it on a range of correlated materials. We compared the properties of different perovskites within three-orbital and five-orbital descriptions, and realized the first GW+DMFT simulations with antiferromagnetic long-range order [4]. Subsequently, the code was extended to a multi-site GW+DMFT framework, which can handle complex materials with several strongly correlated atoms within the unit cell (Fig. 1). This code was successfully applied to the recently discovered nickelate superconductor $Nd_{1-x}Sr_xNiO_2$, where this parameter-free scheme can reproduce all the experimentally known trends, and allowed us to make predictions on the Hall conductivity and other observables [5]. Over the past 6 months we also spent a substantial amount of time on the complete rewriting of the GW+DMFT code, which is now independent of the ALPS and TRIQS libraries, and contains a more efficient impurity solver. This makes it much easier to install the code on different computing platforms, share it with other groups, and eventually release it as an open source code.

In parallel to this theoretical work, the PSI group used the high oxygen-gas pressure setup (P_{max} = 2000 bar) employed during phase 1 to grow the first nickelate single crystals [6]. We focused in particular on the region of the phase diagram where T_{MIT} approaches zero, which we were able to access in $Pr_{1-x}La_xNiO_3$ solid solutions ($0 \leq x \leq 1$). After determining the critical La concentration needed to stabilize a purely metallic state, we employed magnetization, heat capacity, resistivity and Hall effect measurements to obtain information about

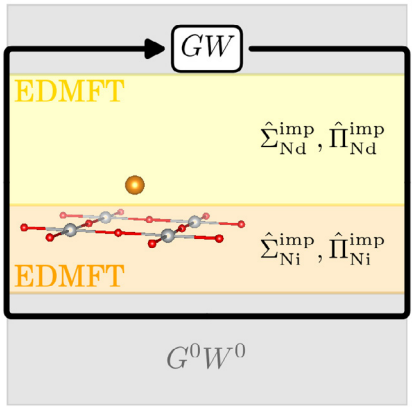

Figure 1: *Schematic illustration of the GW+DMFT self-consistency loop for $Nd_{1-x}Sr_xNiO_2$, with two coupled impurity problems for Nd and Ni.*

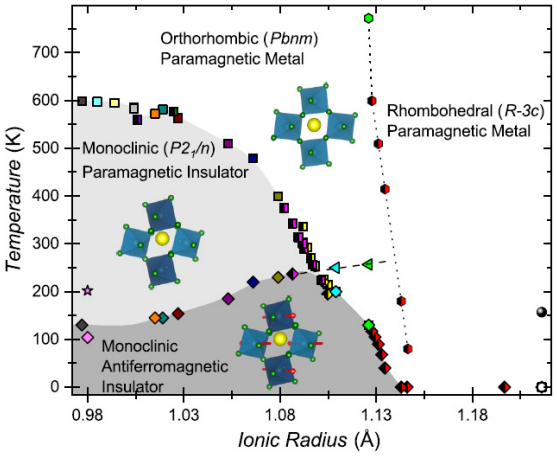

Figure 2: *Updated phase diagram of $RNiO_3$ perovskites.*

the entropy of the MIT, the electron scattering mechanism(s) and their evolution about across the $T_{MIT} = 0$ limit. This information could only be obtained by combining the transport and magnetic data with structural information, obtained from neutron and X-ray diffraction measurements as a function of temperature conducted at the PSI large scale facilities (powder diffractometers DMC and HRPT @ SINQ, Materials Science Beam Line @ SLS). These data enabled the precise determination of the magnetic, metallic and insulating phase fractions as a function of temperature for each one of the samples investigated, a crucial information for the interpretation of the transport data. The obtained results will enable a detailed comparison with the developed theoretical methods that successfully reproduced the transport data reported for superconducting $Nd_{1-x}Sr_xNiO_2$.

PSI also started to investigate the lattice and electron-lattice energy scales and their evolution by approaching the $T_{MIT} = 0$ limit, where both energy scales are expected to become comparable. In order to evaluate the role of the lattice in the MIT, as previously predicted by our calculations [1], we exchanged the oxygen isotope (mostly ^{16}O in natural oxygen) by heavier ^{18}O. This resulted in a substantial T_{MIT} increase (+8.5 K for $PrNiO_3$), which grows in an approximately exponential way with x by approaching the $T_{MIT} = 0$. The analysis of the transport measurements, aimed to evaluate the impact of the O isotope substitution in the electronic mobility, is in progress.

Another important outcome was the precise determination of a second line in the $RNiO_3$ phase diagram corresponding to the metallic I (*Pbnm*) to metallic II ($R\bar{3}c$) phase transition at T_{OR} (Fig. 2). The 1^{st}-order nature of this transition could be unambiguously established. Moreover, we also found that the $T_{MIT} = 0$ and $T_{OR} = 0$ points occur in a very narrow compositional range. This adds an additional degree of freedom to the modeling of this *per se* extremely complex region. It will be also relevant for the interpretation of transport data in thin films, where detailed structural information is difficult to obtain.

Our theoretical and experimental work provides a concise picture of the coupling between electronic, structural, and magnetic properties in the nickelate series, highlighting the role of the electron-electron interaction and in particular the Hund's coupling for the underlying physics. We have now started to explore similar physics also in other materials classes, such as alkaline earth ferrites and chromites. Since the former requires to consider the full five orbital d shell, we have first established the basic phase diagram of such a five orbital Hubbard model including a realistic cubic crystal field splitting, and have already confirmed the presence of a charge-disproportionated insulating phase for realistic interaction parameters, consistent with previous work on two-orbital and three-orbital models. The physical properties of chromate thin films such as $SrCrO_3$ will be investigated by the experimental group of SNSF Prof. Marta Gibert that recently (May 2020) joined the D&D5 project in the frame of an Agility Plus grant.

1.2 Correlated oxide heterostructures

Continuing our phase 1 efforts, the ETHZ group has studied charge transfer phenomena and finite size effects in various transition metal oxide heterostructures. In particular, we demonstrated the formation of a metallic interface between the two Mott insulators $LaTiO_3$ and $LaVO_3$, which is driven by the "electronegativity difference" between the Ti^{3+} and V^{3+} cations [7]. The thickness of the metallic layer in this system can be varied by controlling the epitaxial strain, which is very promising for a potential application as a Mott transistor. In contrast, the metallic character of the $LaVO_3/SrVO_3$ interface is very robust due to the nominal mixed valence of the V cation at the interface. This allows to include specific doping-layers (by including single Sr-O layers in a $LaVO_3$ heterostructure), or potentially also to vary the metallicity of the $SrVO_3$ layers by incorporating strain or reducing the layer thickness. Related $LaVO_3/YTiO_3$ Mott insulating heterostructures were investigated for so-

lar cell applications using non-equilibrium calculations [8]. In collaborative work between ETHZ und UniFR, it was shown that so-called Hund excitations can lead to carrier multiplication in photo-excited multi-orbital systems, which results in an efficiency that potentially exceeds the Shockley-Queisser limit for semiconductor devices.

The interplay between strain, layer thickness, and specific interfacial effects was also studied for $CaVO_3$, in combination with two typical substrate materials, $SrTiO_3$ and $LaAlO_3$. While bulk $CaVO_3$ is a correlated metal, our calculations show that a metal-insulator transition can be induced either via tensile strain or by going to ultrathin films [9]. While $SrTiO_3$ can induce a substantial amount strain in $CaVO_3$, it otherwise acts as an electronically inert substrate, and even reduces the finite size effects compared to free-standing layers [10]. In contrast, $LaAlO_3$ can give rise to interfacial doping, which however depends crucially on the specific electrostatic boundary conditions, allowing for further tunability for various applications.

1.3 Defects in correlated oxides

Electronic structure calculations of point defects in transition-metal oxides are challenging due to the simultaneous need (i) for advanced methods to capture correlation effect combined with (ii) the need for large cell sizes to avoid unrealistically high defect concentrations that lead to artifacts in the energetic and electronic properties of defects. Our work in phase 2 addresses both of these challenges. The team at ETHZ is exploring the computationally demanding DFT+DMFT approach for defects, which allows for an advanced treatment of correlation effects, in particular for systems where electrons are at the border between localized and itinerant. The developed physically intuitive computational scheme allows to specifically study the localization/delocalization of the defect state by explicitly incorporating it in the correlated subspace of the DFT+DMFT calculation. For the prototypical Mott insulator $LaTiO_3$, our calculations show that oxygen vacancies, unexpectedly, do not act as dopants, and thus the Mott insulating state is surprisingly robust against the incorporation of such defects [11]. For $SrTiO_3$, our calculations reveal a subtle balance between localization and delocalization of the electrons released by the vacancy, which is controlled by the strength of the electron-electron interaction both on the Ti d orbitals and the vacancy state. As a result, the system can be tuned between having either one or two electrons localized on the vacancy site. In the first scenario the second electron is delocalized and dopes the Ti d bands. Our cRPA calculations of the screened interaction parameters give a sizable U value for the vacancy orbital, indicating the importance of an explicit treatment of correlation effects also for these states. These results serve as a benchmark for the computationally cheaper self-consistent DFT+$U(+V)$ approach developed for defects at UniBE, which enabled significantly larger cell sizes. While U values were routinely determined in an empirical fashion, our approach computes them self-consistently and around defects that break the translational symmetry also in a site-dependent fashion. Applications to $SrMnO_3$ showed an improved description of the defect energetics [12]. We also established that for partially covalent materials such as $SrTiO_3$ an extended self-consistent site-dependent DFT+U+V scheme is required [13] that, in addition to intra-site, includes also inter-site interactions. This scheme was found to provide defect formation energies with an accuracy comparable to the hybrid functional HSE06, however at a fraction of the computational cost. Importantly, the self-consistent DFT+U+V scheme also yields an electronic structure comparable to sophisticated DFT+DMFT calculations performed at ETHZ.

After this validation of the DFT+$U(+V)$ approach we turned to applying it to design novel defect-induced functionality in transition metal oxides. Using self-consistent DFT+U for oxygen-deficient $LaMnO_3$ [14], we discovered a highly unusual excess-charge accommodation caused by relaxations around the oxygen vacancy in the Jahn-Teller distorted crystal. This arrangement is not inversion-symmetric and leads to a non-zero polarization, the magnitude of which we estimate to be comparable to conventional ferroelectrics such as $BaTiO_3$. Since multiple symmetry-equivalent excess-charge accommodation patterns exist, oxygen vacancies in Jahn-Teller distorted materials could be a novel route towards defect-engineered ferroelectricity. We also applied the self-consistent DFT+U scheme to polar $Fe'_{Mn} - V^{\bullet}_{O}$ and $V''_{Sr} - V^{\bullet\bullet}_{O}$ defect-pairs in $SrMnO_3$. In particular the latter — due to the stronger dipole compared to the former — induces a polar distortion within a sphere of approximately 1 nm diameter. Due to this large strain field, calculations have to be performed in 320 atom supercells, for which sampling the configurational space is only feasible with self-

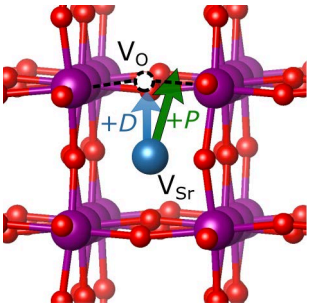

Figure 3: *Alignment of the total polarization **P** in a 320 atom $SrMnO_3$ supercell with the defect dipole **D** created by a $V''_{Sr} - V^{\bullet\bullet}_{O}$ defect pair.*

consistent DFT+*U* (Fig. 3). Based on our calculations, polar defect pairs can hence, at sufficiently high concentrations, induce a polar state in nominally non-polar transition metal oxides, offering an exciting route to engineer ferroelectric and multiferroic materials that we will continue for the remainder of phase 2.
For experimental work performed at PSI, a postdoc was hired, who started to work on perovskite heterostructures that contain a highly ordered two-dimensional network of line dislocations at the interface, building a moiré pattern. From the theory side, we will adapt this to one-dimensional defect structures, which opens a door for the search of novel electronic and magnetic properties within or triggered by the low dimensional ordered network.

1.4 Non-equilibrium formalisms

Apart from the previously mentioned collaboration on Mott solar cells, the UniFR group successfully completed ARPES related projects by a former MARVEL postdoc [15, 16]. These works demonstrated that the circular dichroism in ARPES can detect Berry curvatures, even in highly non-thermal states, and that this provides a powerful tool to track light-induced topological states of matter [16]. We also released the open source library NESSi (non-equilibrium systems simulation package) [17] after several years of intensive coding effort.

MARVEL publications

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

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Design & Discovery 6 Search for Novel Topological Materials

Project leader: Oleg Yazyev (EPFL, 1.75MC)

Computational partner: Titus Neupert (UZH, 1.2MC),
Experimental partners: Ming Shi (PSI, 0.65MC + 0.65MC from PSI), Hugo Dil (EPFL), Christian Rüegg (PSI, EPFL, ETHZ), Arnaud Magrez (EPFL), **Ana Akrap** (UniFR, Agility Plus, 0.8MC)

1 Progress of the different efforts

Project D&D6 aims at the discovery of novel topological materials and the development of associated computational tools. Particularly important results have been achieved in the extension of topological classification of materials, understanding graphene-based topological moiré superlattices and along several experimental directions. Since the beginning of phase 2 our project has resulted in 1 publication in *Science*, 2 in *Nature Physics*, 5 in *Physical Review Letters* and numerous other publications.

1.1 Extension of topological classification

The core activity of project D&D6 aims at establishing a more comprehensive and complete topological classification along with the physical consequences and material realizations. A particularly successful direction of research that involves both computational groups exploits the idea of non-Abelian band topology, largely driven by Tomáš Bzdušek (currently Ambizione fellow in the group of Titus Neupert). We showed that non-Abelian topological charges can be used to characterize nodal-line band degeneracies in metals with space-time inversion (PT) symmetry and weak spin-orbit coupling [1]. The non-Abelian charges put strict constraints not only on the possible nodal-line configurations, but also on their transformations. This analysis goes beyond the standard approach to band topology and implies the existence of one-dimensional topological phases not present in previously proposed classifications. Our more recent work reveals that in Weyl semimetals with C_2T symmetry pairs of Weyl points with opposite chiralities can be stable against annihilation due to the non-trivial Euler number [2]. The topological charges of the Weyl points are transformed according to the braid phase factors, i.e., the annihilation process is path-dependent (Fig. 1b). Our first-principles calculations predict that such braiding of Weyl nodes can be realized in ZrTe and TaAs.

We have recently refined the notion of what is topologically trivial by introducing the concept of delicate topology, which refers to atomic limits with Wannier functions that cannot (due to a topological obstruction) be restricted to a single unit cell. This concept was initially illustrated on Hopf insulators [3]. We have also investigated the possibility for the Hopf insulator to possess localized Wannier representation and the existence of its topological obstructions. We propose that Wannier functions are exponentially localized and preserve the symmetries of the system. Furthermore, we have shown that the surface states of the Hopf insulator phase can be gapped out by surface potential without violating the symmetry or closing the bulk gap. The surface states were shown to have a non-trivial first Chern number that equals to the bulk Hopf invariant [4]. Our study also gives hints regarding possible mate-

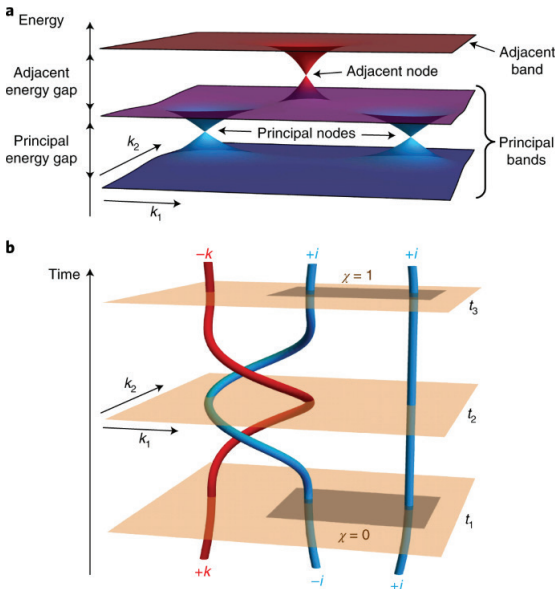

Figure 1: *(a) Schematic representation of a three-band setup with two types of degeneracies necessary for defining the Euler number. (b) Illustration of the braiding process of Weyl nodes.*

rials realizations of this topological phase.
Further progress in extending the classification of topological band degeneracies to include composite Weyl fermions beyond the minimal chiral charge $\chi = \pm 1$ has been achieved. We developed a simple algorithm to identify and classify singular and critical points on Fermi surfaces. This approach allows to explore the classification of the band degeneracies according to the topology of the energy dispersion. Two new type-II band degeneracies with $\chi = \pm 2$ giving rise to exotic Lifshitz transition have been found. We have also started studying the physical consequences of these new types of band crossings, in particular their density of states and chiral Landau levels, as well as searching for the materials hosting these new composite Weyl fermion quasiparticles.

1.2 Materials design: twisted graphene

Recent discovery of the superconducting and correlated insulator phases in twisted bilayer graphene (TBG) has put forward the twist degree of freedom as a new paradigm for designing physical systems with novel properties. The combination of materials design, correlation and topology in twisted heterostructures of 2D materials has created attractive opportunities for the computational partners of project D&D6 given their expertise. Since high-level atomistic calculations on such systems are often impossible due to large sizes of moiré supercells, both groups focused on the development of effective models.
In particular, the group of Neupert developed a symmetry-respecting 12-band tight-binding model that provides an accurate description of the flat-band manifold and the neighboring remote bands in TBG in the non-interacting regime. Furthermore, the computed effective electron-electron interactions for this model enable future studies of the interacting systems. First results on the fractional quantum Hall phase in this system using the DMRG techniques have been obtained. The group of Yazyev has been focusing on lattice relaxation effects, intrinsic crystal field and polarization effects as well as the Hofstadter butterfly physics in TBG and related systems. In particular, the intrinsic polarization effect revealed in twisted *double* bilayer graphene (TDBG) allowed accurate tight-binding description of this more complex moiré superlattice [5]. This progress allowed to join efforts with the group of Guangyu Zhang resulting in the first experimental study of TDBG [6]. This work has revealed several novel properties of TDBG that

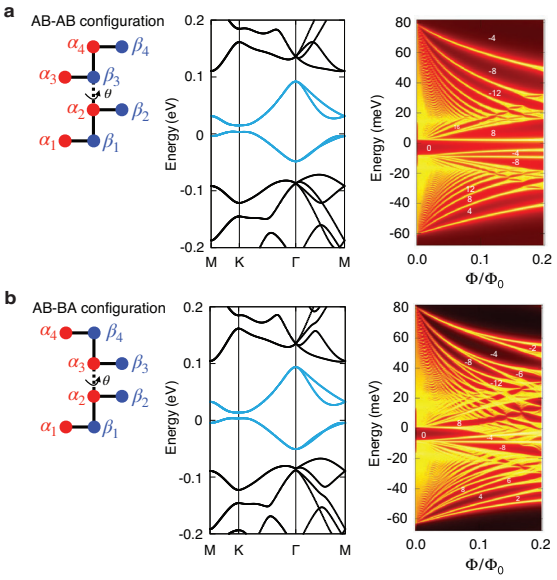

Figure 2: *Two distinct stacking configurations (a) AB-AB and (b) AB-BA of twisted double bilayer graphene. The band structures (middle column) at twist angle $\theta = 1.89^\circ$ are very similar, while the difference in the valley Chern numbers result in different Landau level spectra (right column).*

distinguish it from the parent TBG system, e.g., the spin-polarized insulating state at the half-filling, attracting considerable attention.
Finally, we have put forward a proposal for probing the band topology of moiré superlattices by means of magnetotransport measurements [7]. Our idea was demonstrated with the help of two distinct stacking configurations of TDBG at the same twist angle, which have practically indistinguishable band structures, but different valley Chern numbers of the flat bands. The different Chern numbers clearly manifest as different Landau level sequences in the Hofstadter butterfly spectra (Fig. 2).

1.3 Correlated spin systems

Spin systems represent another class of correlated materials considered in our project, which nevertheless require a distinct theoretical framework. The expertise possessed by the project participants allows accurate evaluation of magnetic exchange couplings by multi-reference quantum chemistry calculations with embedding. The primary objective is the search for novel quantum spin liquid (QSL) materials with a particular focus on candidates realizing the Kitaev model. So far, we identified several candidate materials: $Na_3Co_2SbO_6$ and $Na_3Co_2TeO_6$ that may realize the Kitaev model scenario in an unusual d^7 electronic configuration, and $YbCl_3$ that would be the first Kitaev material among the $4f$-electron sys-

tems. Our configuration interaction calculations revealed a significant magnitude of Kitaev interaction, and experimental efforts to synthesize these candidates and find structurally similar materials in this family has begun (crystal growth facility led by Arnaud Magrez).

Our multi-reference wavefunction calculations have also clarified the supersuperexchange mechanism of exchange interactions in $Sr_2CuTe_xW_{1-x}O_6$, a square lattice double perovskite material possibly hosting a tunable QSL phase. This work was performed in collaboration with experimentalists and published in *Physical Review Letters* [8]. Our multi-reference calculations have also allowed establishing the reference value of Heisenberg exchange parameter $J = -1.44$ meV in single-layer CrI_3 [9], an extensively investigated 2D magnetic material.

1.4 Development of open-source codes

The participants of project D&D6 are actively developing several open-source software projects. WannierTools has become a post-processing tool of worldwide popularity that is capable of evaluating topological indices, surface-state spectra, Berry phase and Berry curvature, identifying topological band degeneracies and many other properties [10]. This code was initiated by Quansheng Wu together with Alexey Soluyanov, and the development continues in the group of Oleg Yazyev. One particularly useful functionality is the highly efficient evaluation of transverse magnetoresistance using the Boltzmann transport approach [11]. It allowed interpreting observations of extremely large non-saturating magnetoresistance (XMR) in a large number of materials, including the topologically trivial α-WP_2 [12] and Weyl semimetal β-WP_2 [11], nodal-line semimetals ZrSiS [13] and MoO_2 [14], SiP_2 [15], and several other materials.

Stepan Tsirkin in the group of Titus Neupert develops software package IrRep [16] that allows extracting the irreducible representations of Bloch states and is compatible with a large variety of first-principle codes. The modern theory of topological quantum chemistry relies on exactly the kind of data that IrRep produces. Furthermore, another major methodological development of Stepan Tsirkin is the WannierBerri code, which is based on a high-performance Wannier interpolation routine [17] and allows to compute with high accuracy linear and non-linear Berry-curvature-related transport responses in materials. An example for the application of this code is [18]. The groups conducted several tutorials and trainings for the users of these codes.

In addition, all participants of project D&D6 develop competence in machine-learning techniques. One example is our recent work on the artificial neural network approach for performing analytic continuation [19].

1.5 Experimental activities

Angle-resolved photoemission spectroscopy (ARPES) remains the main experimental tool in the discovery of novel topological materials, hence the work performed by the group of Ming Shi is of special importance for project D&D6. Since the beginning of phase 2 a large number of important results have been obtained. Firstly, the ARPES investigation of WP_2, the robust Weyl semimetal discovered by us previously [20], has been concluded. Our ARPES measurements confirm the predicted Weyl semimetal phase and unveil the Weyl points that originate from the splitting of 4-fold degenerate band-crossing points with Chern numbers $C = \pm 2$ induced by the crystal symmetries. The manuscript reporting these results has been published in *Physical Review Letters* with the Editor's Suggestion distinction [21]. Another experimental work of the group of Ming Shi in collaboration with two other experimental participants of D&D6 (A. Magrez and H. Dil) addressed the Lifshitz transition in the candidate Weyl semimetal T_d-$MoTe_2$ [22]. The group of Ming Shi has also investigated a particularly rich in terms of physics magnetic topological material $EuCd_2As_2$. It was observed that the degeneracy of Bloch bands is lifted already in the paramagnetic phase of $EuCd_2As_2$ leading to Weyl nodes [23]. Another work explored how the deviation of local magnetic moments that breaks the C_3 rotation symmetry results in a novel state containing three different types of topological phases: axion insulator, topological crystalline insulator, and higher-order topological insulator [24]. Two more publications carried out with active involvements of the computational participants of D&D6 are currently under review. One of them reports the ARPES observation of excitons in the quasi-one-dimensional topological material $TaSe_3$. The other studies PtGa and reports the first experimental observation of Weyl points that go beyond the Nielsen-Ninomiya no-go theorem, i.e. do not have a partner of opposite chirality due to the absorption of Berry curvature by the

Weyl nodal walls.

The experimental capabilities of our project have been considerably extended by the addition of Ana Akrap (UniFR), who joined after receiving an Agility Plus grant in March 2020. Her main experimental techniques are infrared spectroscopy and Landau-level spectroscopy at very low energies, which will be applied to studying magnetic topological materials.

Our project continues extending the scope of collaborations with experimental groups outside the MARVEL community. For example, our expertise in magnetotransport phenomena has resulted in several publications with experimental groups in China and Croatia (see previous section). We would like to highlight specially our recent paper that revealed several types of topological band degeneracies (Kramers-Weyl, composite, and accordion-like Weyl fermions) and associated complex spin textures in chiral crystals of tellurium [18]. Members of both computational groups of project D&D6 made crucial contributions to this work.

2 Contribution to overall goals and initial proposal

Overall, project D&D6 is making steady progress towards the main objectives of the NCCR related to the discovery of novel topological materials and method development activities. Some of the specific plans defined in the phase 2 full proposal, for instance related to the search for novel topological phases and spin systems, proceed with no significant changes. Deviations from the initial research plan are mostly due to changes related to project participants. The initially planned research on device-scale simulations did not see much progress due to the definitive departure of Matthias Troyer. The members of the group of Alexey Soluyanov were accommodated by the group of Titus Neupert, but this did not results in any dramatic modifications of the research program. A research direction on graphene-based moiré superlattices has been added to the program of our project as this field provides interesting opportunities both as an emerging paradigm for materials design and a fertile ground for investigating correlated and topological phases. All participants contribute to introducing machine-learning techniques to their research.

3 Collaborative and interdisciplinary components

Since the beginning of phase 2 we established numerous new collaborations with both theory and experimental groups outside MARVEL, at different institutions in Europe, USA and China. The project also profited from horizontal cooperations with other D&D projects within MARVEL. A visiting Master student (Shiyu Deng) from the group of Nicola Spaldin (D&D5) has carried out a project in the group of Oleg Yazyev on the crystal structure search of novel bismuth halide topological materials (publication in preparation). Another spontaneous project with the group of Alfredo Pasquarello (D&D4) allowed acquiring new expertise [25]. The group of Yazyev has established a close collaboration with the experimental group of Roman Fasel (D&D3) on electronic transport and topological aspects of graphene nanoribbon junctions.

As far as the interdisciplinary component is concerned, the project relies on numerous collaborations with experimental groups to complement its core theory and computational research. The own capabilities of experimental participants of D&D6 cover the majority of work related to materials synthesis ARPES and (magneto)optical measurements, while other types of experimental activities are done by the collaborators outside MARVEL.

MARVEL publications

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

- [1] Q. Wu, A. A. Soluyanov, and T. Bzdušek, *Non-Abelian band topology in noninteracting metals*, Science **365**, 1273 (2019).
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Incubator 1 Design and Discovery of Novel Solid-State Ionic Conductors

Project leader: Teodoro Laino (IBM, 1MC)

Computational partners: Nicola Marzari (EPFL, 1MC)
Experimental partners: Daniele Pergolesi (PSI, 1.3MC + 1.3MC from PSI)

1 Progress of the different efforts

In phase 2, we have consolidated the expertise acquired during phase 1 regarding method and cognitive platform development, computational screening, first-principles techniques and experimental synthesis/characterization, to design and discover novel solid-state electrolytes (SSEs) to promote all-solid-state solutions for next-generation energy storage technologies. The pinball model, direct output of phase 1 (EPFL) [1], was exploited to screen the best 130 ion-conducting structures among 1300 candidates, which were later studied by first-principles techniques. By relying on this screening, which was published in a high-impact journal during phase 2 [2], we were successful in synthesizing, fully characterizing and theoretically validating two promising oxide-based SSEs, $Li_{3+x}Ge_xP_{1-x}O_4$ and Li_7TaO_6, resulting in two publications in field-relevant journals [3, 4]. Starting from the experimental knowledge acquired from the study of $Li_{3+x}Ge_xP_{1-x}O_4$, we authored a review on pulsed laser deposition (PLD) for microbatteries [5]. Moreover, through first-principles techniques, we predicted a previously unreported and highly conductive SSE ($Li_{10}GeP_2O_{12}$ in a tetragonal phase [6]), for which detailed experimental characterization is ongoing at PSI. We provided a computational tool for analyzing the electrochemical stability of SSEs, tested it on various Li- and Na-conductors relevant for all-solid-state batteries (ASSBs), and published the findings in a leading sustainable chemistry journal [7]. We developed and tested a training protocol (IBM) to address Li-ion diffusion in SSEs based on a deep neural network architecture, which was published in an interdisciplinary high-impact journal [8]. We developed a novel method (EPFL) to perform site analysis of molecular dynamics trajectories for ionic diffusion in solids [10]. We presented a methodology to model Li-ion transport in partially delithiated structures, in order to suggest materials whose diffusion properties can be improved by the creation of vacancies through doping [9]. Our tools to obtain paramount SSE properties from molecular dynamics simulations (EPFL) and our AiiDA workflows for evaluating electrochemical stability windows and force-field fitting (IBM) were made public under GitHub repositories (github.com/lekah/samos and github.com/zrl-aiida-toolbox). The landmark analysis published in [10] was also made public as part of SITATOR (github.com/Linux-cpp-lisp/sitator), an open-source Python framework for analyzing networks of sites in molecular dynamics simulations.

All these phase 2 achievements were the subject of several oral contributions at international conferences and can be found in the Materials Cloud open repository for research data. At present, research is ongoing on $Li_{3+x}Ge_xP_{1-x}O_4$ and two beyond-oxide material systems (sulfides, fluorides) from our screening portfolio [2] and from [11, 12]. The next-generation screening of structures with reduced Li-ion stoichiometry and/or partial occupancy is under progress.

The work done in phase 2 also serves as the basis for intense external collaboration, promoting knowledge and technology transfer which is at the heart of NCCR. Thanks to the expertise built in phase 2, Solvay has started a collaboration project with EPFL on SSEs in 2019, and the Materials Cloud will provide the infrastructure for the computational data and simulation services of BIG-MAP (www.big-map.eu), the largest effort in the European Battery 2030+ initiative, with a 2020-2030 timescale.

We detail below the key assets of our research in phase 2, by listing the novel materials reported, the methodologies developed and their open-science solutions.

1.1 Design and discovery of novel materials

The oxide $Li_{3+x}Ge_xP_{1-x}O_4$ $Li_{3+x}Ge_xP_{1-x}O_4$ (LGPO), from the LISICON family of superionic conductors, was chosen early in year 5, after the computational screening [2] predicted its room-temperature conductivity (σ_{RT}) to be

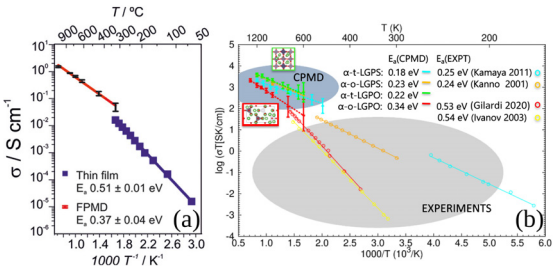

Figure 1: *(a) Arrhenius plot of thin film α-o-LGPO (IS at PSI) and its perfect crystal (FPMD at EPFL) [4]. (b) Arrhenius plot of α-o- (red) and α-t- (green) LGPO from FPMD, with LGPS and experiments [6].*

in the range of one of the most conductive SSEs, $Li_{10}Ge_2P_4S_{12}$ (LGPS, $\sigma_{RT} = 1.2 \times 10^{-2}$ S/cm) [13], if in the same *P42/nmc* tetragonal phase (α-t-LGPO). At PSI, LGPO ceramic pellets were synthesized and shown from X-ray diffraction (XRD) to be *Pnma* orthorhombic (α-o-LGPO), as in [14], with moderate $\sigma_{RT} \sim 10^{-6}$ S/cm. Since this σ_{RT} is in the range of microbattery electrolytes (e.g., LIPON), late in year 5, PSI successfully grew partially crystalline α-o-LGPO films via PLD at RT, which is appealing for commercial manufacturing. In years 5 and 6, first-principles Car-Parrinello molecular dynamics (FPMD) simulations were conducted (EPFL) at constant volume (NVT) at 600−1400 K for bulk α-o-LGPO. The non-full agreement between experimental (pellet and thin film) and FPMD-computed (perfect crystal) σ_{RT} (Fig. 1a) suggested a blocking effect due to large-scale defects. The combined PSI-EPFL efforts on α-o-LGPO resulted in a paper published in year 7 [4]. From variable-cell (NPT) FPMD simulations on α-o-LGPO and LGPS, the elastic moduli were calculated (EPFL) in year 6, with the resulting paper now under submission. In year 6, EPFL also performed FPMD NVT simulations on the hypothetical α-t-LGPO, whose σ is reported in Fig. 1b with both LGPS and experimental results: α-t-LGPO resulted to be a new promising oxide SSE, the study being submitted for publication late in year 7 [6]. The quest for a better Li-conducting oxide motivated a new study, starting year 6: NPT FPMD simulations were conducted at high temperatures (EPFL) to investigate possible entropy-driven phase transitions of α-o-LGPO (*Pnma*) to α-t-LGPO (*P42/nmc*). The transition of α-o-LGPO to a new tetragonal phase (denoted as β-t-LGPO) occurred at 1200 K (Fig. 2a). At PSI, thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC) were employed on an α-o-LGPO pellet, suggesting a phase transition (Fig. 2b) at 700°C The full

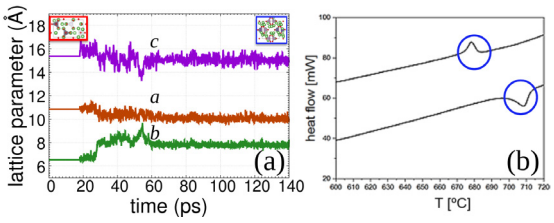

Figure 2: *(a) α-o-LGPO lattice parameters in 1200 K-NPT FPMD (EPFL), showing the transition from α-o-LGPO to β-t-LGPO. (b) DSC on α-o-LGPO (PSI), showing a phase transition at $T \sim 700°C$.*

analysis of this experimental finding is ongoing. This work will be the subject of a joint paper (EPFL-PSI) on the possible new phase(s) for LGPO and their relevance for ASSBs.

The oxide Li_7TaO_6 For Li_7TaO_6 (LTaO), the second material chosen from the screening [2], the experimental study started at PSI early in year 5. Ceramic pellets of LTaO, undoped and aliovalently substituted with Mo^{6+} and Zr^{4+}, were structurally, electrically and electrochemically characterized at PSI through XRD, IS and cyclic voltammetry (CV), respectively. In Q4 year 5, spark plasma sintering significantly improved pellet density and increased σ_{RT}. Further densification and σ_{RT} improvements occurred with Zr^{4+} doping while the opposite effect was observed with Mo^{6+} doping. In the same period, FPMD simulations (EPFL) showed LTaO to be a fast ionic conductor with a ∼0.3 eV diffusion barrier. Early in year 6, IBM fit the parameters of a classical polarizable force field (PFF) to accurately reproduce DFT-PBE reference data via a low-computational approach [3], allowing simulations with longer time/length scales. The Arrhenius plot of the PFF-computed σ is reported in Fig. 3. In Q4 year 5, X-ray photoelectron spectroscopy (XPS) showed that LTaO reacts with CO_2 in the atmosphere, forming Li_2CO_3

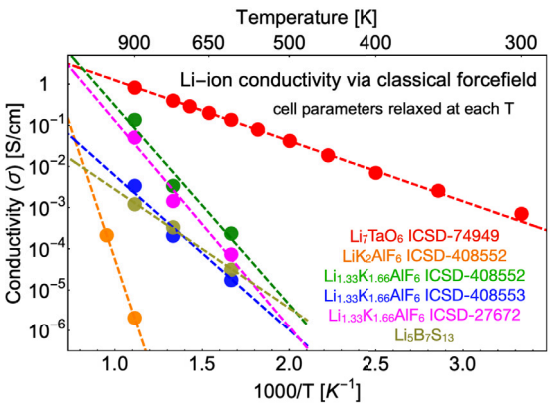

Figure 3: *Li-ion conductivity computed via PFF.*

on the surface (PSI). DFT calculations of the LTaO$-CO_2$ reaction energetics were thus conducted at IBM. The IBM-calculated [7] oxidation and reduction potentials were 2.5 V and 0.3 V vs Li/Li$^+$, respectively, in good agreement with the onset potentials (2.7 V and 0.7 V) experimentally observed (PSI). This collaborative study on LTaO resulted in a paper published early in year 7 [3].

The sulfide Li-B-S system Late in year 6, two thioborate materials were selected for characterization from MARVEL [2] and other [11, 12] computational screenings: $Li_2B_2S_5$ (orthorhombic, space group *Cmcm*) and $Li_5B_7S_{13}$ (monoclinic, space group *C12/c1*). Early in year 7, crystalline phases were obtained by high-temperature solid-state synthesis in inert atmosphere [15]. From IS analysis, started mid-year 7, $Li_2B_2S_5$ did not show significant σ up to 80°C, whereas $Li_5B_7S_{13}$ possessed moderate $\sigma_{RT} \sim 4 \times 10^{-6}$ S/cm. The first result was at variance with FPMD preliminary results (EPFL) conducted in Q2 year 7, that predicted $Li_2B_2S_5$ to be highly conductive ($\sigma_{RT} \sim 10^{-2}$ S/cm). The second result was in agreement with the moderate σ_{RT} computed at IBM for $Li_5B_7S_{13}$ (Fig. 3) by using a force-field potential as in [3]. Ongoing NVT and NPT FPMD simulations will hopefully clarify the conductivity of $Li_2B_2S_5$ and the role of softness in this sulfide structure, which possesses planes of boron and sulfur atoms easily distorted during the dynamics. Also, PSI recently observed evaporation of sulfur during synthesis, suggesting future syntheses using excess sulfur and subsequent simulation insights.

The fluoride LiK_2AlF_6 The study of LiK_2AlF_6 (LKAF) was encouraged by PSI late in year 6, as this superionic material [12], predicted to have a large stability window (up to 5.5 V vs Li/Li$^+$) [12], can be manufactured by an easy and scalable wet-chemistry method [16]. Experimental synthesis plus structural (XRD) and morphological (SEM) analyses started at PSI in Q4 year 6. A study on doping LKAF with LiCl started in Q2 year 7, where ball milling enabled particle size reduction and improved pellet density (Fig. 4c-d). IS analyses of different doping concentrations resulted in the σ values shown in Fig. 5. By increasing LiCl concentration, σ_{RT} increased to $\sim 5 \times 10^{-4}$ S/cm for 25 mol% LiCl-doped LKAF, exceeding the σ requirement for SSEs. For the electronic conductivity σ_e, the (un)doped LKAF pellets showed similar values ($10^{-8} - 10^{-7}$ S/cm) to the well-known LLZO. By XPS analysis (PSI), (un)doped LKAF samples were

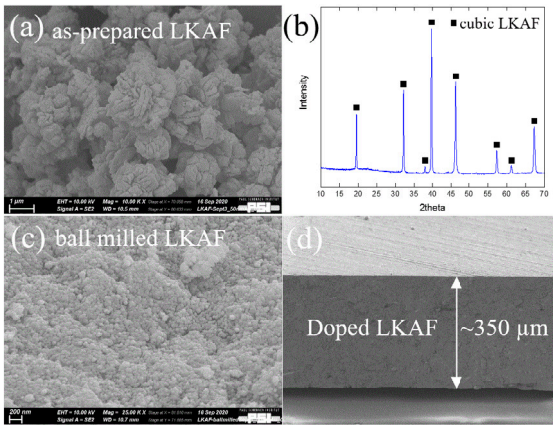

Figure 4: *(a) SEM image of micron-sized LKAF particles from wet chemical synthesis. (b) XRD of the phase pure, cubic LKAF. SEM images of (c) ball-milled LKAF powder without LiCl and (d) cross-section of a ~350 µm thick LiCl-doped LKAF pellet.*

stable up to one hour in air. Using our phase stability tool [7] (IBM), a wide electrochemical stability was calculated in Q3 year 7 for undoped LKAF. Experimental validation by CV is ongoing (PSI). IBM applied the same PFF-based approach used for LTaO [3] to LKAF and its Li-rich ($Li_{1.33}K_{1.66}AlF_6$) and Cl-substituted forms, showing that the superionic σ in doped LKAF originates from the creation of a Li-rich phase (Fig. 3). High-resolution powder diffraction measurements at the MS beamline and inductively-coupled plasma spectroscopy are planned at PSI to elucidate the precise lattice parameters, stoichiometry and phase of the doped LKAF compounds. Additionally, extensive FPMD simulations will be performed on (un)doped LKAF (EPFL). The ongoing experimental and computational explorations are also guided by DFT formation energy calculations of divalent dopants (Mg^{2+}, Ca^{2+}, Sr^{2+})

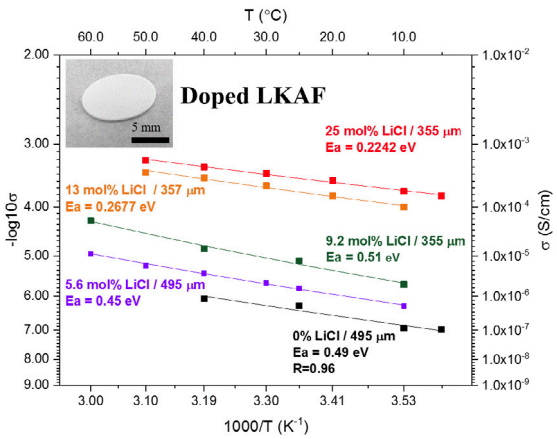

Figure 5: *Arrhenius plot of ball-milled LKAF with various LiCl doping concentrations (0 - 25 mol%).*

on Li^+, K^+ and Al^{3+} sites (EPFL). Sr^{2+} is deemed the most promising dopant, as it substitutes K^+ instead of Li^+, which leads to the formation of K^+ vacancies and further reduction of σ_e. The synthesized LKAF consisted of micron-sized agglomerates with a cubic crystal structure (Fig. 4a-b).

1.2 Conceptual, methodological and algorithmic developments

Materials screening (EPFL) Our pinball-based [1] high-throughput screening of Li-containing insulators without partial occupancies and at full stoichiometry ended mid-year 6 and was published later that year [2]. In year 6, we performed a second screening by removing 20% of Li content in the materials, suggesting the best 12 structures to PSI for synthesis. In year 7, a third screening effort was directed toward materials with partial occupancies, exploiting the electrostatic energy as a proxy to find low-energy configurations. We are currently developing a structural screening with both reduced Li-ion stoichiometry and partial occupancies.

Electrochemical stability (IBM) A systematic study of state-of-the-art computational methodologies to evaluate electrochemical stability windows (ESWs) started at IBM in year 5. The outcome was the development of a tool (published during year 7 [7]) to evaluate ESWs of SSEs using two complementary methodologies (the *grand potential phase diagram method* and the *method of stable stoichiometry*).

Neural networks for force fields (IBM) A training protocol to address Li-ion diffusion in SSEs based on a deep neural network architecture and PFFs was developed at IBM in year 6 and published in year 7 [8].

Landmark analysis of sites (EPFL) In year 5, a novel approach to detect the relevant events in a diffusive system without assuming prior information (unsupervised landmark analysis) was developed and tested on some of the best SSEs; the results were published in year 6 [10].

Doping analysis (IBM) In year 5, the complex interplay between doping and conductivity was clarified through an approach (based on the analysis of PFFs trajectories) able to capture and distinguish thermodynamic and kinetic effects due to the insertion of a dopant in a pristine material. The results were published in year 6 [9].

Elastic moduli from MD (EPFL) In year 6, the method of strain fluctuations to compute elastic moduli from MD trajectories was applied to SSEs for the first time (EPFL). The results are being drafted in a publication and will be made public within a GitHub repository.

1.3 Open Science: codes, data, tools, and workflows/turnkey solutions

Electrochemical stability AiiDA workflow
github.com/zrl-aiida-toolbox/zrl-aiida-toolbox (IBM-EPFL)

Fitting of force fields AiiDA workflow
github.com/zrl-aiida-toolbox/fitter (IBM-EPFL)

MD simulations post-processing
github.com/lekah/samos (EPFL)

Landmark analysis for Li-ion diffusion
github.com/Linux-cpp-lisp/sitator (EPFL)

2 Contribution to overall goals and initial proposal

The primary goal of this MARVEL Incubator is the discovery of novel SSEs for next-generation batteries. In phase 2, we identified and characterized five unreported solid-state electrolytes, developed new methodologies for materials screening as well as electrochemical and conductivity analysis, and leveraged the AiiDA and Materials Cloud infrastructures, which are central elements for simulation automatization and data dissemination. Within the overall aims of NCCRs, MARVEL Incubator 1 has established close ties between multiple Swiss institutions (EPFL, IBM, PSI) and contributed to knowledge and technology transfer outside MARVEL (Solvay, BIG-MAP, Belenos, REPSOL partnerships).

3 Collaborative and interdisciplinary components

In MARVEL phase 2, we established an intense collaboration around promising candidate materials outputted from the EPFL screening. These have been studied experimentally (synthesis, characterization) at PSI and tested computationally (Car-Parrinello FPMD, PFF, our own developed methods) at EPFL and IBM. Two workflows developed by IBM were made available through AiiDA turnkeys thanks to the collaboration with EPFL. The most promising potential SSEs from these joint experimental and computational studies have been manufactured at PSI. Ways to improve technolog-

ically important material properties (e.g. doping for improved ionic conductivity/stability) were also proposed by PSI and exchanged with EPFL/IBM in biweekly meetings to further refine the computational efforts and complete the synergistic feedback loop. A highlight of the extensive collaborative spirit of the project has been the mobility of researchers between EPFL, PSI, and IBM, with e.g. Aris Marcolongo, Leonid Kahle, and Tobias Binninger having being hired at different times by two of the three partners involved. Additionally, thanks to the expertise acquired in phase 2, paramount external partnerships were built: in year 6, Solvay has started a collaborative project with EPFL on SSEs, and the Materials Cloud will provide the infrastructure for the computational data and simulation services of BIG-MAP (www.big-map.eu), the largest effort in the European Battery 2030+ initiative.

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. Kahle, A. Marcolongo, and N. Marzari, *Modeling lithium-ion solid-state electrolytes with a pinball model*, Physical Review Materials **2**, 065405 (2018).
- [2] L. Kahle, A. Marcolongo, and N. Marzari, *High-throughput computational screening for solid-state Li-ion conductors*, Energy & Environmental Science **13**, 928 (2020).
- [3] L. Kahle, X. Cheng, T. Binninger, S. D. Lacey, A. Marcolongo, F. Zipoli, E. Gilardi, C. Villevieille, M. E. Kazzi, N. Marzari, and D. Pergolesi, *The solid-state Li-ion conductor Li_7TaO_6: A combined computational and experimental study*, Solid State Ionics **347**, 115226 (2020).
- [4] E. Gilardi, G. Materzanini, L. Kahle, M. Döbeli, S. Lacey, X. Cheng, N. Marzari, D. Pergolesi, A. Hintennach, and T. Lippert, *$Li_{4-x}Ge_{1-x}P_xO_4$, a Potential Solid-State Electrolyte for All-Oxide Microbatteries*, ACS Applied Energy Materials **3**, 9910 (2020).
- [5] L. Indrizzi, N. Ohannessian, D. Pergolesi, T. Lippert, and E. Gilardi, *Pulsed Laser Deposition as a Tool for the Development of All Solid-State Microbatteries*, Helvetica Chimica Acta **104**, e2000203 (2021).
- [6] G. Materzanini, L. Kahle, A. Marcolongo, and N. Marzari, *Electrolytes for Li-ion all-solid-state batteries: a first-principles comparative study of $Li_{10}GeP_2O_{12}$ and $Li_{10}GeP_2S_{12}$ in the LISICON and LGPS phases*, arXiv:2010.08068 (2020).
- [7] T. Binninger, A. Marcolongo, M. Mottet, V. Weber, and T. Laino, *Comparison of computational methods for the electrochemical stability window of solid-state electrolyte materials*, Journal of Materials Chemistry A **8**, 1347 (2020).
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Incubator 2 — Active Machine Learning for Computational Materials Design

Project leader: Anatole von Lilienfeld (UniBas, 1MC)

Computational partners: Volker Roth (UniBas, 0.5MC), Michele Ceriotti (EPFL), Martin Jaggi (EPFL)

1 Progress of the different efforts

Activities directly related to MARVEL have included several research projects since May 2018.

1.1 Revision of FCHL representation

In order to enhance the applicability and usability of our quantum-machine-learning models we have mainly focused on a revision of the FCHL representation, published in 2018 (FCHL18) [1]. While the use of FCHL18 within kernel ridge regression based machine-learning results in highly competitive predictive accuracy, its computational efficiency decays rapidly for larger training set sizes. We have alleviated the computational burden by using a discretized version of a Fourier series expansion fitted to the interatomic three-body terms in FCHL18. Fig. 1 illustrates this effect for two angles in the water molecule. Training timings for the resulting new FCHL model (FCHL19) [2] on training sets consisting of 1000 different snap-shots drawn from MD data for various organic molecules are also shown in Fig. 1. Comparison between FCHL19 and FCHL18 models indicates potential CPU time savings of one order of magnitude.

Due to its superior computational efficiency, more extensive hyper-parameter optimization runs of FCHL19 based machine-learning models are possible. This can result, for some datasets, in vastly superior predictive power. In the case of predicting the binding energy in clusters with sum formula $(H_2O)_{40}$, for example, learning curves indicate that the advantageous hyperparameters of FCHL19 enable predictions twice as accurate after training on ∼1500 geometries (Fig. 2). Thanks to the Operator approach [3], energies and forces can now be efficiently modeled (crucial for molecular dynamics or geometry relaxation of larger systems), and are always among the top 3 methods in terms of predictive power for systems that have been studied in the literature (Fig. 2).

1.2 Role of gradients

We have studied the role of gradients in the loss functions for training and testing, respectively. Numerical results indicate that for machine-learning models of the potential energy surface of any given system, the inclusion of forces in the loss function of training is beneficial for the accuracy of energy predictions. When training and predicting across chemi-

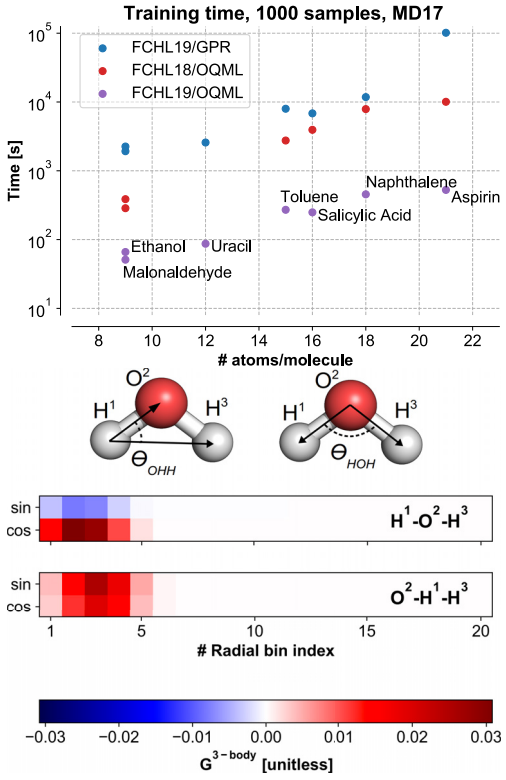

Figure 1: *Methodological illustrations for FCHL19 [2]. Top: training timings for kernels of rank 1000 with three different methods for ethanol, malonaldehyde, uracil, toluene, salicylic acid, naphthalene, and aspirin. Timings are calculated as averages over 5 kernels using different random splits on a 24-core node equipped with two Intel Xeon E5-2680v3 @ 2.50 GHz CPUs. Bottom: the three-body basis functions are plotted for the two unique three-body terms in the water molecule, corresponding to the O2-H1-H3 and H1-O2-H3 angles displayed at the top. The atoms are numbered for clarity.*

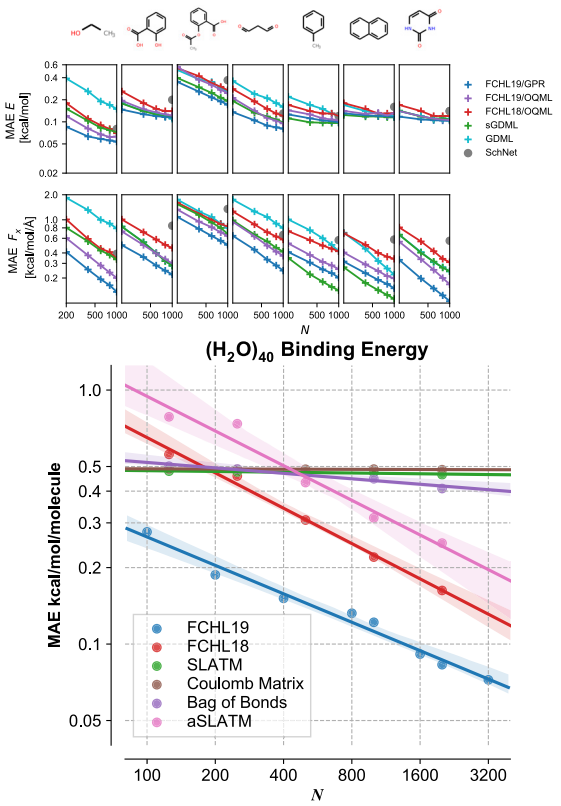

Figure 2: *Performance illustrations for FCHL19 [2] Top: learning curves for various machine-learning models predicting forces and energy for snapshots of 7 molecules from the MD17 dataset. The first and second row refer respectively to energy (E) and force component (F) mean absolute errors (MAE) for out-of-sample predictions. Bottom: learning curves for the Water40 dataset: The mean absolute error (MAE) binding energy per molecule is plotted for 6 different representations versus the training set size. Linear fits are displayed for clarity, and shaded areas denote the 95% confidence intervals for the fits as obtained via boot-strapping.*

cal compound space, however, the inclusion of forces in the loss function of training has negligible benefit for energy predictions. As one would expect, the accuracy of force predictions improves in either case. By now, this work has been submitted, peer-reviewed, and published [4].

1.3 Deep latent archetypes

In this research project we developed a method for representing molecules as convex combinations of extremal (or *archetypal*) molecules [5, 6] with respect to certain properties. The proposed method extends classical linear archetypal analysis (AA) to nonlinear variants by employing sophisticated deep neural networks within an encoder-decoder framework. Unlike the original formulation, this deep AA model is generative and capable of handling physico-chemical side information of molecules. We empirically demonstrated the applicability of our approach by exploring the chemical space of small organic molecules from the QM9 datasets. In doing so, we found two different latent archetype representations with respect to specific molecule properties like atomisation energy, band-gap energy and heat capacity. We are convinced that this type of partly supervised exploration of the chemical space has the potential to advance the field of *de novo* molecular design in a significant way.

1.4 Inverse learning of symmetries

The goal of this research project was to describe invariances induced by symmetry transformations with the help of deep latent variable models. In complex domains such as the chemical space, invariances can be observed, but usually the underlying symmetry transformation cannot be formulated analytically. We have developed a machine-learning model to estimate such symmetry transformations from observations. For this purpose, we use two latent subspaces, where the first subspace captures an observable chemical property and the second subspace the remaining invariant information encoding structural variations of molecules that do not change the property of interest. In a recent publication [7] we showed that this model was capable of learning structural variations molecules that are invariant with respect to both band-gap energies and polarisabilities. The generative nature of this model made it possible to find new molecules not contained in the training data, with specified properties (Fig. 3). We are currently working on extending this model in such a way that the precise 3D-structure of molecules can be generated directly [8].

1.5 Other efforts

Independently, we have also studied the application of machine-learning methods to the (i) modeling of X-ray powder diffraction, (ii) melting and boiling points of molecules, and (iii) energetics of conformational isomers. Unfortunately, the team member working on the first project decided to stop her PhD studies. Manuscripts reporting on projects (ii) and (iii) will be submitted soon.

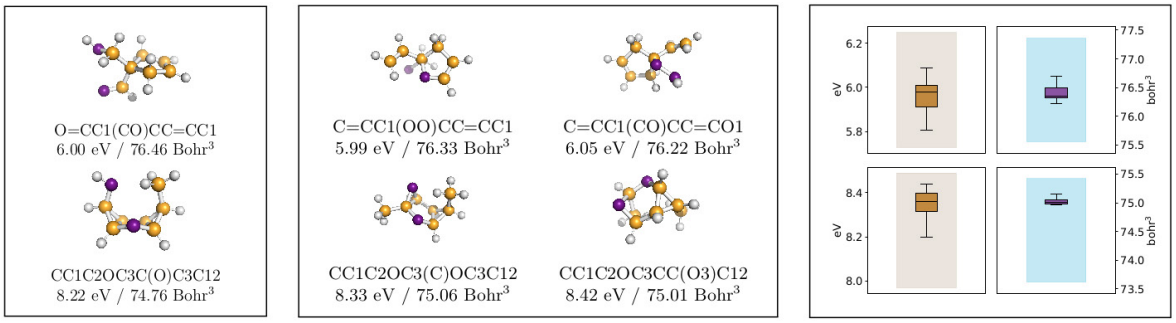

Figure 3: *Panel (a) shows the reference molecules which serve as our starting point with their corresponding properties. In (b), we plotted two generated molecules which are closest to the reference molecule. The properties from the generated molecules are estimated by using the prediction network of our model. Additionally, we predict the properties of all generated molecules (approx. 37 per point) and depict them as a box plot in (c), where the left box plot denotes the band gap energy and the right box plot the polarizability. The cross shaded background is the confidence interval.*

2 Contribution to overall goals and initial proposal

As specified in the phase 2 full proposal, the work of this incubator serves to further the development and implementation of machine-learning models for the wider sake of the overall MARVEL effort. In order to facilitate usage by other MARVEL teams, we have open sourced our developments at github.com/qmlcode/qml. Manuals and documentation have also been made available at qmlcode.org.

3 Collaborative and interdisciplinary components

In order to support the organic crystal research in Design & Discovery project 1, we have assessed the performance of kernel ridge regression models based on the FCHL representation [1] for the modeling of non-covalent interactions. More specifically, corrections to the density functional SCAN for the prediction of van der Waals interactions in common benchmarks have been studied. By now, this work has been peer-reviewed and published [9].

MARVEL publications

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

- [1] F. A. Faber, A. S. Christensen, B. Huang, and O. A. von Lilienfeld, *Alchemical and structural distribution based representation for universal quantum machine learning*, The Journal of Chemical Physics **148**, 241717 (2018).
- [2] A. S. Christensen, L. A. Bratholm, F. A. Faber, and O. A. von Lilienfeld, *FCHL revisited: Faster and more accurate quantum machine learning*, The Journal of Chemical Physics **152**, 044107 (2020).
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- [4] A. S. Christensen and O. A. von lilienfeld, *On the role of gradients for machine learning of molecular energies and forces*, Machine Learning: Science and Technology **1**, 045018 (2020).
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- [6] S. M. Keller, F. Arend Torres, M. Samarin, M. Wieser, and V. Roth, *Exploring Data Through Archetypal Representatives*, in *to be published in NeurIPS 2019 Workshop on Learning Meaningful Representations of Life Workshop* (Vancouver, 2019).
- [7] M. Wieser, S. Parbhoo, A. Wieczorek, and V. Roth, *Inverse Learning of Symmetries*, in *Advances in Neural Information Processing Systems 33 pre-proceedings (NeurIPS 2020)*, H. Larochelle, M. Ranzato, R. Hadsell, M. Balcan, and H. Lin, eds. (Curran Associates, Inc., 2020), Neural Information Processing Systems.
- [8] V. Nesterov, M. Wieser, and V. Roth, *3DMolNet: A Generative Network for Molecular Structures*, arXiv:2010.06477 (2020).
- [9] P. D. Mezei and O. A. von Lilienfeld, *Noncovalent Quantum Machine Learning Corrections to Density Functionals*, Journal of Chemical Theory and Computation **16**, 2647 (2020).

Open Science

Open Science Platform

Project leader: Giovanni Pizzi (EPFL)

Computational partners: Nicola Marzari (EPFL), **Michel Kenzelmann** (PSI)

1 Progress of the different efforts

1.1 AiiDA

Work on AiiDA has focused on improving stability, robustness and efficiency, with the 1.0 release in October 2019, followed by releases improving robustness and providing new key features. Two papers have been published: the full overview of the AiiDA 1.0 infrastructure [1], published in *Nature's Scientific Data*, and a technical one on the details of event-based workflow engine [2]. A survey conducted in April 2020[1] received responses on 69 AiiDA-powered research projects at different stages of completion, 36 of which already published (11 in 2017-2018, 25 in 2019-April 2020), showing the rising impact of AiiDA in materials science research. AiiDA users have contributed to many new open plugins and workflows, resulting in a 3.4× growth of plugin packages in the AiiDA plugin registry[2] (from 17 in May 2018 to 58 in December 2020).
On the technical side, a new event-based workflow engine has been implemented, integrated with an improved provenance model clearly separating data and logical process units. AiiDA now supports 10'000+ computations/hour, and provides users with introspection tools for analyzing the provenance graph (Fig. 1). It also now deals seamlessly with node failures and network issues via automatic reattempts and pause fail-safes. Automated error handling for workflows was introduced to address issues such as computation timeouts and advanced convergence logic. Automatic data migration ensures that data collected with earlier versions of AiiDA remain compatible and reusable. All improvements were made while observing a strict testing regime, with 1000+ new tests written, in order to guarantee a smooth user experience.
An efficient local object store implementation has been developed, reducing the load on the file system for large-scale high-throughput applications with 100'000+ calculations. Combined with a new archive format, it delivers orders of magnitude faster importing, exporting and backing up of AiiDA databases. The prototype implementation is now in the testing phase and slated for the next major release in spring 2021.
An important ongoing effort is to deliver common interoperable workflows[3] to run the same simulation (e.g. crystal relaxation) transparently with many codes (currently involved: Abinit, BIGDFT, Castep, CP2K, FLEUR, Gaussian, NWChem, Orca, QUANTUM ESPRESSO, SIESTA, VASP).

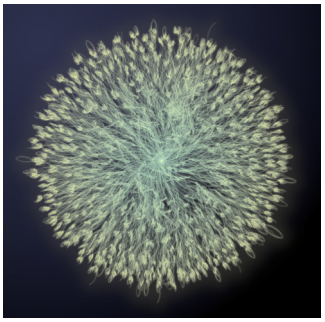


Figure 1: *AiiDA provenance graph with ∼100'000 nodes, representing the workflows to assess carbon capture performance, applied to 324 covalent-organic frameworks [3].*

1.2 Materials Cloud, AiiDAlab, Quantum Mobile

a) *Materials Cloud* Since its launch in February 2018, Materials Cloud has been growing steadily, absorbing learning materials, simulation tools, and data archives, as well as attracting new visitors with roughly 15k unique monthly visits in November 2020. Materials Cloud is now also a GO FAIR[4] implementation network, promoting FAIR data principles in computational materials science and beyond. A detailed summary of the architecture, its main achievements, and its philosophy going forward can be found in the recently published article [4] in *Nature's Scientific Data*.
We now describe the progress of each section. The 56 new lecture recordings added

[1] www.aiida.net/science
[2] aiidateam.github.io/aiida-registry
[3] github.com/aiidateam/aiida-common-workflows
[4] www.go-fair.org/

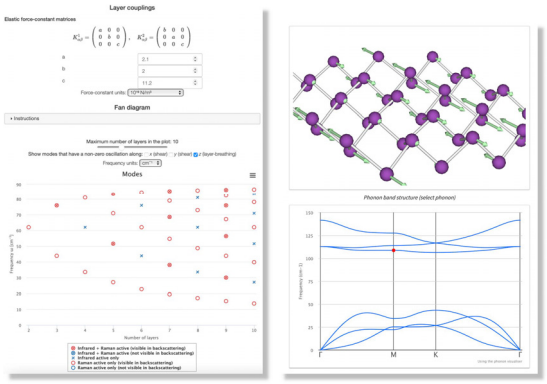


Figure 2: *Two Materials Cloud tools. (Left) Tool to compute fan diagrams and optically-active modes of layered materials. (Right) Tool to interactively display normal phonon modes.*

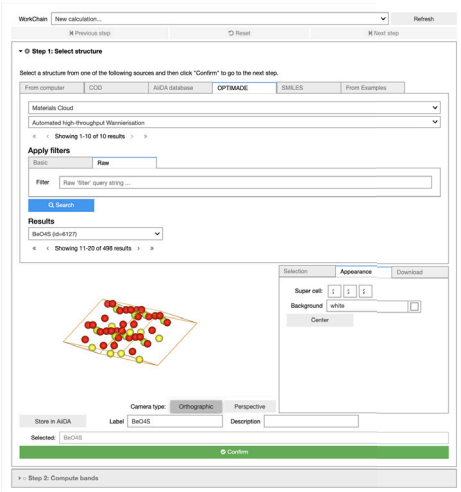


Figure 3: *AiiDAlab* QUANTUM ESPRESSO *application interface. The input structure can be taken from multiple sources; here, from Materials Cloud using the OPTIMADE client (optimade.org).*

to the *Learn* section since May 2018 include MARVEL distinguished lectures, CECAM-MARVEL Classics in molecular and materials modeling, CECAM-MARVEL Mary Ann Mansigh conversations, videos from the Wannier90 v3.0 school and AiiDA tutorial lectures, as well as Nicola Marzari's "Fireside chats for lockdown times", which reached hundreds of listeners live and thousands via the recording.

Submissions to the Materials Cloud *Archive* have taken off substantially from ≈30 in 2018 to more than 150 in 2020 (over 250 total). *Nature's Scientific Data* now recommends the Materials Cloud *Archive* as a repository for materials science data, and the repository is indexed in services such as Google Dataset search and B2FIND. The repository is now starting to attract submissions from research groups worldwide. To support this rapid growth, the *Archive* section has been moved to the scalable Invenio 3 (the backend of Zenodo, developed at CERN) providing users with free-text search, personal user accounts with integrated moderation workflows, and record history tracking. This transition enables the *Archive* to take advantage of new features developed by the large Invenio community, and it simplifies the process of on-boarding new moderators.

Materials Cloud has grown to host many highly curated dataset, now counting 13 *Discover* sections in December 2020, from many different MARVEL projects. Each of these sections hosts the corresponding data on the Materials Cloud *Archive*, and the majority of them has the corresponding simulations data, run with AiiDA, directly browsable and downloadable in the corresponding *Explore* sections, with interactive access to the full provenance graph.

Materials Cloud also hosts scientific tools to perform computations directly in the browser (Fig 2). Researchers from various MARVEL projects and from outside MARVEL have started contributing to several tools (10 tools available in 2020 vs 1 in May 2018, gathering over 40% of the unique visits to Materials Cloud). To ease the on-boarding of new tools, we switched to the dokku platform-as-a-service (PaaS) backend, making it easy for contributors to (i) write new tools by leveraging common templates ("buildpacks") and (ii) test/update existing tools by a streamlined git integration.

b) *AiiDAlab and Quantum Mobile* Work on AiiDAlab has been mostly focused on increasing the stability of the service, transitioning to a scalable Kubernetes backend, making it easily redeployable, and developing user-friendly AiiDAlab applications and tools to streamline new apps development. The design of the platform is described in [5], together with 3 applications used in production at Empa in a mixed experimental/theoretical laboratory. To enable the use of the platform by a broader community, we have setup an open AiiDAlab instance[5] with login open to any academic researcher (via the EOSC Hub/EGI authentication service). One of the main goal of AiiDAlab is to provide the infrastructure where computational scientists can build and share scientific tools in a form of users-friendly web apps like the one of Fig. 3. Being tightly integrated with AiiDA workflows, AiiDAlab apps offer a way also for non-experts to prepare and submit advanced simulations (running on supercomputers) directly in the browser. To ensure the

[5] aiidalab-demo.materialscloud.org

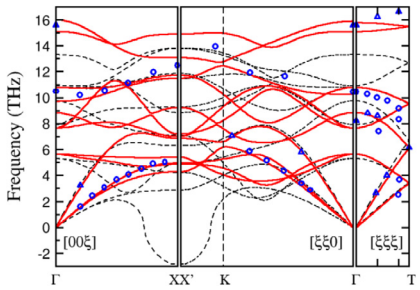
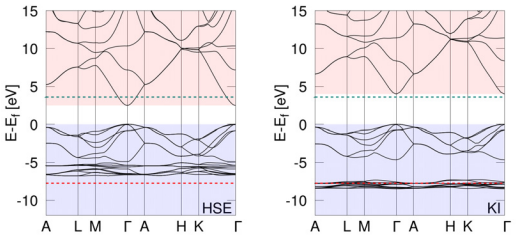


Figure 4: *Comparison of the vibrational spectra of CoO as computed using DFPT (black dashed lines), DFPT+Hubbard (red solid lines), and as measured in inelastic neutron scattering experiments (blue open circles and triangles).*



	HSE	G_0W_0	scGW̃	KI	Exp.
E_{gap}	2.48	3.0	3.2	3.98	3.60
$\langle\varepsilon_d\rangle$	-5.95	-6.4	-6.7	-7.9	-7.75

Figure 5: *HSE and Koopmans (KI) band structure of ZnO. Shaded areas highlight valence (light blue) and conduction (light red) manifolds. Table: band gap and position of Zn d states (in eV) with respect to the top of the valence band at different level of theory compared to experimental and scGW̃ results.*

stability of the apps (as their number steadily grows) we developed an AiiDAlab test action[6], allowing developers to test new changes before they get released on AiiDAlab (e.g., mimicking user's behavior and clicks, and checking if the results are expected).

Quantum Mobile has been developed as a virtual machine solution for providing a uniform environment for quantum-mechanical simulations. Quantum Mobile includes a wide range of open-source quantum mechanical simulation codes, ready to be used either directly or through AiiDA. Since May 2018, Quantum Mobile has been used in 10+ workshops and tutorials both within and outside MARVEL and has been downloaded more than 10'000 times, with extremely positive feedback both from students and lecturers.

1.3 Computational spectroscopies and microscopies and curated data

a) *Vibrational spectroscopies* We have developed, implemented, and applied Hubbard-corrected density-functional perturbation theory (DFPT+Hubbard) with the atomic Hubbard manifold and *ab initio U* for calculations of phonon vibrational spectra of transition-metal compounds [6] (Fig. 4). We have extended the ground-state formalism to orthogonalized atomic Hubbard manifolds, and derived and implemented the calculation of Hubbard forces and stress based on the exact solution of the Sylvester equation [7]. Moreover, we generalized the DFPT formalism to inter-site Hubbard V interactions (crucial for balancing hybridization versus localization), in the ultrasoft and projector-augmented-wave formulations, and extended it to metallic ground states [8]. These developments have been released open-source with QUANTUM ESPRESSO v.6.6 and are currently used for simulations of phonon spectra in rare-earth nickelates, in collaboration with the experimental group of Marisa Medarde at PSI.

b) *Photoemission spectroscopies* During phase 2, we mainly focused on the implementation of Koopmans' spectral functionals in QUANTUM ESPRESSO as a reliable tool for accurate and efficient photoemission spectroscopies simulations. The approach was extended to take advantage of the translational symmetry in crystals, leading to a formalism suitable for periodic-boundary-condition codes. The bare and screened Koopmans' corrections are decomposed in monochromatic contributions, one for each **q**-point in the Brillouin zone (BZ) of the primitive cell, and efficiently evaluated using DFPT plus a sampling of the BZ. As a natural consequence, a band structure picture is automatically recovered (Fig. 5). During the last year we also worked on the integration of the Koopmans' code with the latest QUANTUM ESPRESSO distribution, as a necessary precondition for an upcoming release.

c) *XAS and RIXS at the K and $L_{2,3}$ edge* Most of the work focused on the methodological development, implementation, and application of the X-ray absorption spectra (XAS) simulation for modeling K-edge spectra of transition metal oxides, in particular pristine and Ni-substituted $LaFeO_3$ [9]. We interfaced the XSpectra code of QUANTUM ESPRESSO with the Hubbard-corrected DFT scheme including the on-site U and inter-site V Hubbard corrections. The U and V parameters are efficiently computed from first principles using our novel

[6] github.com/aiidalab/aiidalab-test-app-action

implementation [10] based on DFPT. During the last year we also explored possible strategies to simulate XAS and resonant X-ray scattering (RIXS) at the $L_{2,3}$ edge of transition metal and rare-earth ions. This can be done fully *ab initio* at the GW+BSE level with the OCEAN code or modeling the crystal field on the emitting atom from the DFT charge density and importing it into an atomic multiplet calculator.

2 Contribution to overall goals and initial proposal

The various components of the Open Science Platform have matured to form a solid basis of a computational infrastructure. AiiDA has grown to be a stable and robust code, with a very broad support of over 50 different simulation packages, used to power tens of already-published research projects and many more to be soon submitted. Combined with very robust and interoperable workflows for materials science, it allows the creation of curated and fully reproducible datasets that can be published on Materials Cloud (data with DOIs in the *Archive*, curated data in the *Discover* section, full provenance in the *Explore* section). With over 200 *Archive* submissions and 13 highly curated datasets as of December 2020, Materials Cloud has become a key platform for dissemination and FAIR sharing of reproducible research results. AiiDAlab provides the environment to develop and run workflows "in the cloud", with minimal setup and making complex HPC workloads accessible also to non-specialists. It accelerates experiment-simulation interactions and, ultimately, materials discovery. The Quantum Mobile virtual machine provides a seamless platform to run schools and tutorials for teaching and education, and has been already used to simplify the setup of tens of events, with extremely positive feedback from teachers and students.

On the computational spectroscopies and microscopies side, ground-state and linear-response DFPT+Hubbard formulations are accurate, automated, user-friendly, and robust tools for simulations of structural, electronic, magnetic, and vibrational properties of complex transition-metal and rare-earth compounds. They are open access via QUANTUM ESPRESSO. The DFT+Hubbard workflow (including self-consistent calculation of on-site U and inter-site V Hubbard parameters) is being integrated in AiiDA. Koopmans' spectral functionals provide a reliable and efficient alternative to more expensive and cumbersome Green's function techniques for the simulation of spectral properties [11, 12, 13]. The release as part of QUANTUM ESPRESSO will make it easily accessible to the scientific community also via AiiDA workflows.

3 Collaborative and interdisciplinary components

Groups from many MARVEL D&Ds are using AiiDA and contributing to AiiDA workflows, publishing their curated datasets on Materials Cloud, and/or making online tools available on Materials Cloud. We have established tight collaborations at the European level with large TIER-0 HPC centres in Europe, with the Battery2030+ project BIG-MAP, with many H2020 projects (the MaX and TREX CoE, Marketplace, Intersect, Dome 4.0, OpenModel). Many international collaborations are also ongoing for the development of workflows for materials science, e.g., with SINTEF Norway (VASP), Microsoft (Wannier90), ICMAB Spain (SIESTA), etc. Collaborations have also been established for the technology needed to deliver interactive educational content: with the OSSCAR project at EPFL and with the executable-books project at Berkeley US.

Furthermore, close collaborations with experimental groups at PSI are ongoing; examples includes (i) the investigation of metal-insulator transition in nickelates (Marisa Medarde), (ii) the calculation of exchange parameters in magnetic systems [14] (Christian Rüegg), (iii) the analysis of structural stability in organic-inorganic multifferoics (Romain Sibille), and (iv) the band structure calculation of heavy fermion systems (Michel Kenzelmann). We also provided support to the EPFL Laboratory of Ultrafast Spectroscopy for the simulation of ARPES and XAS spectra of lead halide perovskites [15].

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. P. Huber, S. Zoupanos, M. Uhrin, L. Talirz, L. Kahle, R. Häuselmann, D. Gresch, T. Müller, A. V. Yakutovich, C. W. Andersen, F. F. Ramirez, C. S. Adorf, F. Gargiulo, S. Kumbhar, E. Passaro, C. Johnston, A. Merkys, A. Cepellotti, N. Mounet, N. Marzari, B. Kozinsky, and G. Pizzi, *AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance*, Scientific Data **7**, 300 (2020).
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- [6] A. Floris, I. Timrov, B. Himmetoglu, N. Marzari, S. de Gironcoli, and M. Cococcioni, *Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials*, Physical Review B **101**, 064305 (2020).
- [7] I. Timrov, F. Aquilante, L. Binci, M. Cococcioni, and N. Marzari, *Pulay forces in density-functional theory with extended Hubbard functionals: from nonorthogonalized to orthogonalized manifolds*, Physical Review B **102**, 235159 (2020).
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- [9] I. Timrov, P. Agrawal, X. Zhang, S. Erat, R. Liu, A. Braun, M. Cococcioni, M. Calandra, N. Marzari, and D. Passerone, *Electronic structure of pristine and Ni-substituted $LaFeO_3$ from near edge x-ray absorption fine structure experiments and first-principles simulations*, Physical Review Research **2**, 033265 (2020).
- [10] I. Timrov, N. Marzari, and M. Cococcioni, *Hubbard parameters from density-functional perturbation theory*, Physical Review B **98**, 085127 (2018).
- [11] N. L. Nguyen, N. Colonna, A. Ferretti, and N. Marzari, *Koopmans-Compliant Spectral Functionals for Extended Systems*, Physical Review X **8**, 021051 (2018).
- [12] 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).
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- [14] F. Giorgianni, B. Wehinger, S. Allenspach, N. Colonna, C. Vicario, P. Puphal, E. Pomjakushina, B. Normand, and C. Rüegg, *Nonlinear quantum magnetophononics in $SrCu_2(B_3)_2$*, submitted (2020).
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HPC

HPC and Future Architectures

Project leaders: Joost VandeVondele (CSCS and ETHZ), **Thomas Schulthess** (CSCS and ETHZ)

1 Progress of the different efforts

The HPC and Future Architectures platform led by CSCS is involved in two major types of activities: (i) support the deployment of the hardware resources for MARVEL (storage space, computing facilities and web-hosting of Materials Cloud) and (ii) software developments in the domain of electronic structure to ensure the effective usage of current and future HPC architectures in the complex scientific workflows.

1.1 Hardware resources

In the past 33 months, the hardware arrangement stayed at a constant level. MARVEL project owns 180 dual-socket compute nodes (2x Intel Broadwell 18-core, E5-2695 v4 @ 2.10 GHz), with 64 GBytes of memory (DDR4 @ 2133 MHz) which are clustered to the multicore partition of Piz Daint and which were utilized more than 90% in the period from May 2018 until November 2020. MARVEL compute nodes have a full access to the scratch filesystem of 2.7 PetaBytes. Besides that, 150 TB of permanent storage is available exclusively for MARVEL. The Materials Cloud infrastructure (web frontend, AiiDA backend and storage) is hosted on the OpenStack instance at CSCS. Around 256 cores, 910 GB RAM and 50 TB of storage are assigned for this service.

1.2 Software developments: SIRIUS library

SIRIUS is a domain specific library developed at CSCS with the purpose of creating a common GPU backend for the plane-wave DFT codes. In phase 1, SIRIUS library was interfaced with QUANTUM ESPRESSO code and tested to work correctly in the AiiDA workflows involving crystal structure relaxation running on GPUs. The SIRIUS-enabled QUANTUM ESPRESSO code is installed as a module on Piz Daint for all users.
In the past 33 months the following developments in the SIRIUS library have been accomplished. First, the iterative Davidson solver was improved in order to use a smaller diagonalization subspace (thus, less memory and smaller eigenvalue problem size) and benefit from wave-functions locking. The locking of the wave-functions allows to exclude converged eigenstates from the subspace search. Second, the stable Anderson mixing algorithm was implemented. In this implementation the least-squares problem is solved using an updated QR factorization, instead of inverting the matrix of the normal equations directly. Third, the mechanism of call-back functions was implemented in order to compute the values of radial integrals of the form

$$I(q) = \int j_\ell(qx) f_\ell(x) x^2 dx \qquad (1)$$

and

$$I'(q) = \int \frac{\partial j_\ell(qx)}{\partial q} f_\ell(x) x^2 dx \qquad (2)$$

using the QUANTUM ESPRESSO implementation for radial integration. In these expressions $f_\ell(x)$ is any of augmentation charge, local potential, beta projectors and non-linear core correction radial functions defined by the pseudopotential and the radial integrals are used to compute corresponding lattice periodic functions or their lattice strain derivatives. This is required to address the issue of numerical reproducibility of SIRIUS-enabled QE with respect to the original implementation. Finally, a lot of effort has been put in the development of the AMD ROCm backend for SIRIUS. The QE-SIRIUS is fully working on AMD GPU cards with one performance issue remaining on the rocBLAS side. This gives a confidence that crystal structure relaxation workflows will be possible to execute on the AMD-based supercomputers (LUMI in Finland, Frontier at ORNL, USA) starting from day zero of the operation.

1.3 Software developments: Robust wave-function optimization

As observed by our collaborators from the THEOS group at EPFL, approximately 10% of magnetic structures fail to converge using the standard SCF density minimization. Direct wave-function minimization methods provide a robust fallback solution.

We have finalized the prototype implementation of the minimizers in Python and implemented the Marzari-Vanderbilt-Payne pseudo-Hamiltonian method in the standalone library `nlcglib` [1] using modern C++. The `nlcglib` is now integrated into SIRIUS and SIRIUS-enabled QUANTUM ESPRESSO. The API of the library has been designed such that it is possible to integrate it into other DFT codes.
The mathematical expressions comprising the wave-function gradient rely either on BLAS/LAPACK routines, e.g., matrix-matrix multiplication, or Cholesky decomposition and eigenvalue solvers, for which we provide wrappers to cuBLAS/cuSolver and MKL. The gradient with respect to the pseudo-Hamiltonian matrix involves also entry-wise operations. In order to deal with these operations and to achieve performance portability we rely on the Kokkos library [2]. Kokkos provides a programming model in C++ for writing performance portable applications targeting all major HPC platforms. In particular Kokkos kernels can run on multi-core architectures (OpenMP/Pthreads backend), Nvidia (CUDA) and AMD GPUs (ROCm).
Currently `nlcglib` runs on multi-core CPUs and Nvidia GPUs, targeting Piz Daint. However adding support for AMD GPUs (to run, for example, on the LUMI HPC system) requires adaptions only in the build system and specializations for the interface to the AMD GPU specific versions of BLAS/LAPACK.
Benchmarks carried out in the THEOS group at EPFL confirmed a success rate of 98% of the `nlcglib` wave-function optimizer on a magnetic test set which failed to converge with standard SCF density minimization.
Comparing performance on Piz Daint, we observe that a single conjugate gradient step is 2–7× faster than the corresponding SCF cycle in the GPU-accelerated SIRIUS (Fig. 1). High speed-ups are possible for cases when the Davidson iterative eigensolver exhibits slow convergence and therefore requires many applications of the Hamiltonian or when the number of SCF iterations is high.
The Python API has been kept up-to-date with the changes in C++ SIRIUS. Generalization to the ultrasoft pseudopotentials is almost complete and will be finished in the coming weeks. In addition to the current API, which is based on functors, e.g., for the application of the Hamiltonian to a wave-function object and inner products, we will provide a state-machine based implementation, which will facilitate integration of our solver with CP2K.

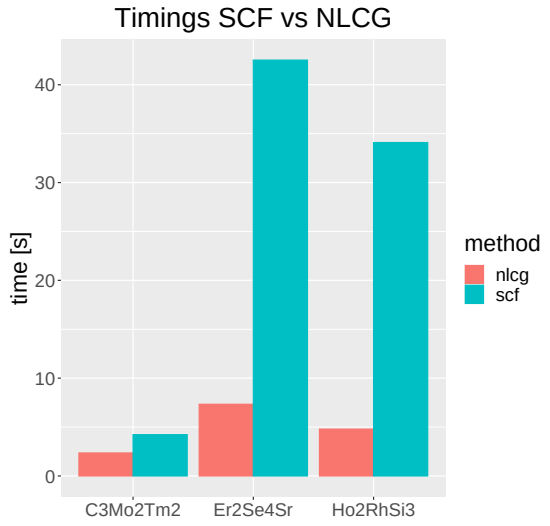

Figure 1: *Wall time of a single conjugate gradient step (nlcg) versus a single SCF iteration (scf). Measurements were carried out on the GPU partition of Piz Daint.*

2 Contribution to overall goals and initial proposal

The work which is done at CSCS serves two purposes: 1) ensure that MARVEL infrastructure (compute, storage, Materials Cloud hosting) is fully functional and available to the users and 2) contribute to the software development and performance portability of the important community codes such as QUANTUM ESPRESSO and CP2K.

3 Collaborative and interdisciplinary components

The work on the software development and performance portability is done in collaboration with the THEOS group at EPFL. This collaboration goes smoothly and we are making a good progress in delivering the robust wave-function optimisation technique in QUANTUM ESPRESSO through the SIRIUS interface. Other components, such as high-performance numerical libraries for CP2K and QE are developed in MaX CoE and PASC with a mutual interest in designing a portable, high-performance scientific software for the research community.

Other references

[1] https://github.com/simonpintarelli/nlcglib.

[2] H. C. Edwards, C. R. Trott, and D. Sunderland, *Kokkos: Enabling manycore performance portability through polymorphic memory access patterns*, Journal of Parallel and Distributed Computing **74**, 3202 (2014).

4.2 New projects

Six new members entered MARVEL in May 2020. Lyndon Emsley (EPFL) joined the D&D1 project as experimental PI through some reallocation of funding within the project and Urs Staub (PSI) joined D&D5 for the second half of the phase, replacing Marisa Medarde (PSI) as already planned in the proposal for phase 2. Moreover, four new female PIs joined MARVEL through the Agility Plus call for projects. These are:

- Sereina Riniker, PATT at ETHZ, on "improving the generation and sampling of crystal packings with machine learning" and integrated in D&D1,
- Emiliana Fabbri, senior researcher at PSI and 2020 PRIMA recipient, on the "search for MOF-based catalysts for the electrochemical splitting of water" and integrated in D&D4,
- Marta Gibert, SNSF professor at UZH, on the "electronic properties of $SrCrO_3$ thin films" and integrated in D&D5,
- Ana Akrap, SNSF professor at UniFR, on "topological materials with intrinsic magnetic ordering" and integrated in D&D6.

Marisa Medarde's project, planned only for the first half of the phase, carried over the first three months of year 7 until the end of July and Michele Parrinello retired at the end of December 2020.

5 Structure-related aspects

The MARVEL activities, actions and achievements carried out in phase 2 in the NCCR's four management areas of knowledge and technology transfer, education and training, equal opportunities, and communication, are presented below. They follow the measures and action plans presented in the strategies for phase 2; any exception is noted in the text. In the last year, some activities were cancelled as a consequence of the COVID-19 crisis, and many other have turned online, with often interesting and positive outcomes, thanks to the imagination and personal initiative of MARVEL members.

5.1 Knowledge and technology transfer

5.1.1 Knowledge transfer

Software

AiiDA

The development of the AiiDA platform, with in particular the release of AiiDA 1.0 in October 2019, is described in the OSP section of the Research chapter. Beside the code development, one major activity is its dissemination through the scientific community and beyond, in particular with international AiiDA tutorials, including in Lausanne (Switzerland), Xiamen (China), Ljubljana (Slovenia), Oslo (Norway), Mandi (India), Tokyo (Japan); the full list is available on www.aiida.net/events. The 2020 edition of the AiiDA tutorial was organised in an entirely virtual format, which gave the opportunity to reach a truly global audience. In total, we accepted 85 participants from 30 countries and 13 different time zones[1] (Fig. 1). Dedicated workshops in 2019 and 2020 helped AiiDA plugin developers migrate to AiiDA 1.0 and take advantage of the new workflow engine (as of December 2020 the AiiDA plugin registry has 58 plugin packages, covering almost 100 code executables). Thanks to dedicated volunteers, the AiiDA documentation has been translated into Chinese[2]. AiiDA has been accepted as an affiliated project of the NUMfocus organisation[3] that promotes open practices in research, data, and scientific computing. AiiDA participated successfully in the 2020 Google Summer of Code, with student contributions improving the compatibility of AiiDA with the Jupyter ecosystem and was presented at the 2020 Scientific Python conference with over 900 participants. The AiiDA community is continuously informed through Twitter and Facebook posts.

Figure 1: *AiiDA annual tutorial, virtual edition, July 2020.*

Materials Cloud

Materials Cloud is central to MARVEL. It is built to enable the seamless sharing and dis-

[1] A detailed report is available at www.aiida.net/report-on-the-2020-aiida-virtual-tutorial

[2] aiida.readthedocs.io/projects/aiida-core/zh_CN/latest/

[3] www.numfocus.org

semination 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 OSP section.
After nearly 18 months of planning and programming, a new Materials Cloud *Archive* was unveiled at the end of May 2020 with a major re-engineering based on the CERN-developed data technology that also drives the massive Zenodo repository. The new archive improves the user experience, provides the scaling needed to accommodate the growing number of submissions and helps moderators and developers focus on the core work of the archive-enabling the seamless sharing and dissemination of resources in computational materials science. Let us note that the *Archive* is used as open data repository for the MARVEL research data management strategy, with about 85 MARVEL-related entries in year 7 and 163 in total.

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. It has been developed to enable the use of the platform by a broader community. In addition, it has been stress tested to scale to at least 50+ users. Quantum Mobile is a virtual machine for computational materials science and provides a uniform environment for quantum mechanical materials simulations. Simulation codes are set up and ready to be used either directly or through the AiiDA python framework for automated workflows and provenance tracking. It has been used in 10+ courses and tutorials, including the AiiDA tutorials or the Wannier90 v3.0 school, virtual edition in March 2020. Details about the developments of both platforms can be found in the OSP section.

New releases, open source codes

Since the beginning of phase 2, new open source codes were released, with, e.g.,

- WannierBerri (wannier-berri.org), a code to calculate different properties by means of Wannier interpolation (2020, Stepan Tsirkin, Neupert group);
- FWP finite-size corrections (github.com/falletta/finite-size-corrections-defect-levels), to calculate the finite-size corrections of total energies and single-particle energy levels involving defect states with built-in ionic polarization in supercell calculations (2020, Pasquarello group);
- NESSi, NonEquilibrium Systems Simulation Library (nessi.tuxfamily.org), to enable efficient and accurate computations based on nonequilibrium Green's function (2019, Werner group);
- Environ 1.1 (www.quantum-environ.org), to handle environment effects in first principles condensed-matter simulations, in particular for applications in surface science and materials design (2019, Marzari and Goedecker groups);
- QML: A Python Toolkit for Quantum Machine Learning (www.qmlcode.org), for representation learning of properties of molecules and solids (von Lilienfeld group).

A detailed list of codes released by the MARVEL community can be found on nccr-marvel.ch/publications/codes.

Collaborations and conferences

Other EU and Swiss synergies

The long-term planning and strategy of MARVEL have made it an ideal partner for shorter-term European projects that share the same vision — so the SNSF investment has allowed to leverage complementary funding from a significant number of projects. As mentioned earlier most notably these are the H2020 MaX Centre of Excellence for Materials Design at the Exascale (max-centre.eu, 2015–2018, 2018–2021), H2020 MarketPlace — Materials Modelling Marketplace for Increased Industrial Innovation (the-marketplace-project.eu) — (2018–2022), aimed at developing a single point of access for materials modeling activities in Europe, and H2020 INTERSECT — Interoperable Material-to-Device simulation box for disruptive electronics (intersect-project.eu) — (2019–2021), driving the uptake of materials modeling software in industry, bridging the gap between academic innovation and industrial novel production, with a goal of accelerating by one order of magnitude the process of materials' selection and device design and deployment; H2020 OpenModel (Integrated Open Access Materials Modelling Innovation Platform for Europe) and DOME 4.0 (Digital Open Marketplace Ecosystem 4.0) are starting in year 7; all of these projects leverage the AiiDA and Materials Cloud IT infrastructure of MARVEL. In addition, strategic efforts have taken place in the Coordination and Support Action that led to the creation of the European Materials Modelling Council, and in the provision of simulation services of the H2020 NFFA

— Nanoscience Fine Foundries and Analysis (nffa.eu) — (2015–2020) and its successor, NEP (NFFA-Europe-Pilot), for the period 2021–2025.
Importantly, MARVEL will provide core data and simulation services for BIG-MAP (Battery Interface Genome — Materials Acceleration Platform), the flagship activity in the newly launched 10-year European action "Battery 2030+".
Clémence Corminboeuf is involved in two Marie Skłodowska-Curie actions, LIDOS (Light-Induced Spin Switch using Dynamic Organic Species) and D3AiSF (Screening Database to Discover Donor-Acceptor copolymers for intramolecular Singlet Fission), Jürg Hutter in one, MOFdynamics (Investigating metal-organic frameworks using excited-state dynamics and theoretical spectroscopy), and Mathieu Luisier in another, CAMPVANS (Investigation of carrier multiplication in van der Waals heterostructures for superlattice for future highly efficient photovoltaic components).
In Switzerland, the support of Materials Cloud by swissuniversities P5 grant (2019–2020) has been renewed and receives additional funding in 2021. The project OSSCAR (Open Software Services for Classrooms and Research) has been launched in 2019, in collaboration with the Centre Européen de Calcul Atomique et Moléculaire (CECAM), of thanks to the EPFL Open Science fund to build an open, collaborative online hub to host simulation and data-analysis tools with an environment that offers software tools as easy-to-use services requiring little or no setup time.

Conferences organized by MARVEL members

Every year, MARVEL members organized or co-organized many conferences, tutorials or workshops, and some are also sponsored by MARVEL. All are listed in the NIRA database and on the website (nccr-marvel.ch/ctw) and since the beginning of phase 2 there are more than 60. Due to the COVID-19 crisis, in 2020, many were cancelled, others turned online and some were inspired by the crisis. As an example of the last category we can mention the "Fireside chats for lockdown times: A gentle introduction to DFT calculations", three two-hour sessions in April 2020 given by Nicola Marzari over Zoom to expose the fundamentals, practical application and the capabilities and limits of the technique. The first session maxed out at the limit of 500 participants before it even got started. The recordings are available on Materials Cloud *Learn*.

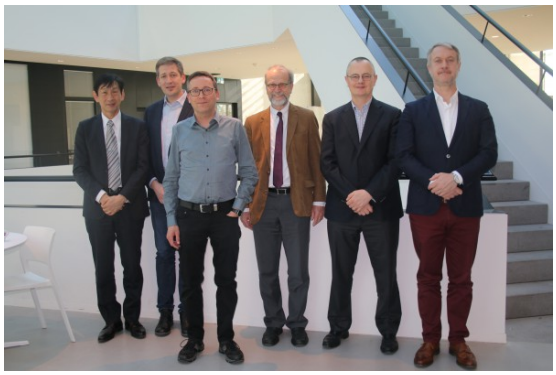

Figure 2: *MARVEL Industrial Advisory Board with from left to right Ryoji Asahi, Arnaud Grandeury, Thomas Eckl, Erich Wimmer, Nicolas Cudré-Mauroux, Frédéric Diologent, February 2020.*

5.1.2 Technology transfer

Industrial Advisory Board

In phase 1, industrial contacts were developed mainly through awareness-raising at events in Switzerland, and by approaching individual companies or in response to spontaneous requests to meet MARVEL PIs. At the beginning of phase 2, an Industrial Advisory Board (IAB) was established that brought 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 (Fig. 2). Two IAB meetings held on September 12, 2018 and February 6, 2020. These discussions drew our attention to the fact that the level of acceptance of computational materials science varies between different industrial sectors, but overall, industry needs broad use of computational tools. The IAB encouraged the formation of precompetitive industrial consortia addressing specific topics. They expressed concern about what will happen after the end of MARVEL since industry needs user-friendly software compatible with existing IT infrastructure with long-term support. Phase 3 involves strategies to achieve this goal.
At the end of the second IAB meeting, an industrial panel discussion about "Working in industry: what you want to know" wa organized for the MARVEL PhD and postdocs (open to EPFL students as well). The six IAB members were involved and the event has gathered 70 participants, leading to many interactions and ending with an aperitif.

Industry sector days

The purpose of the sector days is, for the MARVEL researchers, to gain insights into the broad needs of industrial enterprises regarding the use of atomic-scale modeling. One main activity of MARVEL is to develop platforms for high-throughput and turn-key computations of material properties and for databases of material properties. The collective input from sector day participants spanning a range of industries should guide the choices for applications of these platforms during phase 3. To reach this goal, we have invited industrial representatives at C-level, senior experts, or innovation managers from large companies by activating industrial contacts gathered during phase 1 or through networks of the IAB, MARVEL PIs, and the EPFL VP for Innovation.

The first sector day **on metals** took place on Feb. 15, 2019 with six European companies, one leader in aluminium metallurgy, two car manufacturers, one leader in aeronautics, one watch-maker and an automotive supplier. The focus was on D&D2, with the participation of two non-MARVEL professors sharing experimental mechanical metallurgy. While participants were impressed with MARVEL activities, the highest interest was in controlling manufacturing and defects, and secondarily Hydrogen embrittlement, which are not well-aligned with direct MARVEL work although efforts are being made by MARVEL PI(s) in other projects.

The second sector day **on pharma and fine chemistry** took place on Oct. 10, 2019 with one food, five pharma and two fine chemistry companies. This sector involves companies for which structure, stability and crystallization kinetics play strategic roles. The focus of the meeting was on D&D1 (crystal structure prediction, machine learning used for modeling of complex molecular crystals and compounds, NMR crystallography platform). Several companies were interested in using a cosortium platform on modeling, but possible collaborations are on hold during the COVID-19 crisis.

The third sector day **on materials for energy** took place on Feb. 7, 2020 with ten companies and five PIs from EPFL, PSI and IBM Research. The focus was on materials for energy production and storage, and related to Incubator 1 (Li compounds for batteries, materials for electrolysers, use of deep neural networks in modeling). In feedback, the industrial panel emphasized the need to expand scope to include transport mechanisms across/in grain boundaries, film formation, composite systems, to collaborate more with experimental researchers and to model defects in materials to approach real conditions.

The fourth sector day **on materials for electronics** took place online on Dec. 4, 2020 with nine companies. The focus was on D&D3 and D&D5 (discovery of novel 2D materials and their investigation as active components of transistors, development of advanced *ab initio* models and their application to metal-insulator transitions in oxide heterostructures, fabrication of graphene- and TMD-based devices). Industrial feedback mentioned the need for a broader range of materials data, not only material compositions and bulk physical properties, but extended to defects, interfaces and surfaces. To tackle industrial issues, a true multiscale approach to bridge atomistic with device engineering would be appreciated and useful.

The fifth sector day **on chemistry & catalysis** took place online on Jan. 14, 2021 with nine companies active in flavor, pharma, nutrition and chemical specialties. In an effort to emphasize and improve gender balance, four of twelve industrial participants were women. The focus was on D&D1 and D&D4 (heterogeneous catalysis, MOFs, AiiDA and Materials Cloud platforms). However, with the new NCCR on Catalysis, MARVEL included PI participants from this new program as well, to help that program launch industrial interactions.

The outcome of each meeting is usually a written document of comments and recommendations that serves as a reference and guide for future MARVEL planning, and also avenues for possible direct engagement with individual companies. Due to the sector days, the IAB, and individual PI efforts, we have a community of 45 large companies that have been exposed to MARVEL research. A long-term vision with the continuation of databases and tools is of interest for all industrial sectors. In phase 3. We will leverage this community to make our platform and databases sustainable and to open new collaborations.

Start-up Matscreen in incubation

Matscreen is a start-up project incubated from Berend Smit's lab. The purpose is to develop an online platform enabling automatic screening of crystalline materials for industrial applications, with a focus is on gas adsorption in nanoporous materials, such as MOFs, COFs and zeolites. MARVEL TT manager coached them to prepare pitch presentations and opened contacts in companies, with the aim to identify possible applications and get industrial case studies to apply their modeling

methods. In 2020, Matscreen met four companies; three showed an interest to continue the discussion and one gave a use case to get better understanding of Matscreen added-value.

Industrial collaborations

Since the beginning of phase 2, MARVEL PIs have obtained about ten significant industrial collaborations with large international companies in collaborations that could not have happen without MARVEL. Funding for these projects in years 5-7 totals more than 3 MCHF for MARVEL years 5-7. Some companies are now proposing extensions of their collaboration, demonstrating long-term interest.

Other activities

A first industrial newsletter was sent out in November 2017 to 80 subscribers. Since then, new editions are sent out in February, June and November, with 286 subscribers by the end of 2020.
Following the IAB's recommendations to make young researchers aware of career opportunities in industry, three visits to industries, including exchanges with industrial researchers, were planned at Novelis, Novartis and IBM Research. Because of the COVID-19 pandemic, these visits could not take place, together with participation to the STI-EPFL industrial day (planned in March) and the ETHZ Industry Day (planned in September).

5.2 Education and training

5.2.1 PhD students and postdocs

In the MARVEL community

In phase 2, we continued to encourage junior scientists to take the lead in interacting and stimulating new collaborations through student-organized summer schools and junior seminars, chaired by PhD students or postdocs.

Junior seminars

MARVEL junior seminars continue taking place monthly. Initially held on campus at EPFL, they have been moved in a virtual format since the first COVID-19 lockdown. They aim to intensify interactions between MARVEL junior scientists from to different research groups. More details are given in the Communication chapter.

Summer schools

As a continuation of the three MARVEL Junior Retreats organized in phase 1 (2015, 2016, 2017), a 4-day retreat took place on July 17–20, 2018 in Fieschertal. The event, organized by two junior researchers, was planned in a workshop style including selected keynote speeches aimed at improving research skills and professional development, and presentations by the participants, carefully chosen to achieve a good balance of research groups, gender, as well as master students, PhDs and postdocs. Other activities were organized in order to foster friendly relations between different groups in the community.

In 2019, a group of MARVEL PhD students organized a summer school entitled "Advanced Electronic Structure Methods in Condensed Matter Physics". The organizers managed to obtain ETH Board funding for the school, and wanted to organize their effort somewhat independently of MARVEL. Because of the 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 rather than organize a competing Junior Retreat. The school took place on July 8–10, 2019 at EPFL and was a big success, attracting 146 participants, including 53 members of current MARVEL groups, and a few more members of phase 1 MARVEL groups. The 3-day school provided an overview of advanced methodologies in computational condensed matter physics. The summer school consisted of lectures given by 14 internationally renowned speakers, many of whom are domain experts from leading international institutes. A doctoral course was associated with the school, offering ECTS credits for students from the ETH domain.
In 2020, a similar arrangement was planned, with the NCCR supporting a summer school organized by MARVEL junior researchers, but the summer school could not take place because of the COVID-19 crisis. The event, remodeled as a workshop entitled "First-Principles Modelling of Defects in Solids" (sites.google.com/view/defects-in-solids) is postponed to June 2-4, 2021, to be held at ETHZ or online if the situation does not allow an in-person event. It will overview the latest

advances in the theory and simulation of defects with a focus on the methodologies developed for the description of defects in the condensed phases, together with their application to technologically relevant systems.

Education platform

Since its launch in 2017, MARVEL intensively uses the *Learn* platform of Materials Cloud (www.materialscloud.org/learn) as educational platform. It was populated with the recordings of the MARVEL distinguished lectures, the CECAM-MARVEL Classics in molecular and materials modeling, the CECAM-MARVEL Mary Ann Mansigh conversations, and this year the Nicola Marzari's "Fireside chats for lockdown times" on DFT calculations, which reached hundreds of listeners live and thousands via the recording.
The platform also hosts the recording of various schools and tutorial lectures, as the AiiDA plugin migration workshop of March 2019, the tutorial on reproducible workflows in computational materials science of May 2019, as well as the virtual tutorial of July 2020 and the Wannier90 v3.0 School — Virtual Edition 2020, in March. This platform, central to MARVEL, is a space for students and experts to gather knowledge and consolidate expertise in the domain of materials simulation.
As a collaboration with CECAM funded by the EPFL Open Science Fund, through the OSSCAR (Open Software Services for Classrooms and Research, osscar.org) platform, the OSP team is developing some of the core tools needed for "computational thinking" and original educational content, offering the infrastructural resources developed for the Materials Cloud, and disseminating widely through the CECAM network and beyond.
Outside of Materials Cloud, during the first spring lockdown, Nicola Spaldin developed teaching material, with three series of modules available on her YouTube channel, "The Beginner's Guide to the Modern Theory of Polarization", "Introduction to Correlated Materials" and "Solid State Physics and Chemistry of Materials".

CECAM/MARVEL Classics in molecular and materials modeling

In 2019, MARVEL and CECAM launched a series of lectures at EPFL on "Classics in molecular and materials modeling". In this series, 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. The two first lectures of the series, with 40–50 participants, were:

- Jean-Paul Ryckaert and Giovanni Ciccotti, April 30, 2019, on "Molecular dynamics under (holonomic) constraints" .
- Michele Parrinello and Roberto Car, July 25, 2019, on "Car-Parrinello molecular dynamics".

Two are planned for the very near future, as online events:

- David Vanderbilt and Raffaele Resta, March 23, 2021, on "Berry phases in condensed matter physics".
- Daan Frenkel and Tony Ladd, in May 2021, about free energies of crystals.

Outside MARVEL

Other schools

MARVEL PIs regularly organize and/or lecture to various schools in the domains of MARVEL, e.g. the yearly MolSim school — Understanding Molecular Simulation — with Berend Smit (online in 2021), or other CECAM schools. MARVEL students are encouraged to participate to these schools. Conferences, tutorials, workshops, and schools organized by MARVEL members are listed on the website (nccr-marvel.ch/ctw).

Initiatives in sub-Saharan Africa

MARVEL supports the African School series on Electronic Structure Methods and Applications (ASESMA). The mentoring and training is led in collaboration with the International Center for Theoretical Physics (ICTP) in Trieste. Since 2010, ASESMA is a bi-annual 2-week school providing an introduction to the theory of electronic structure, with an emphasis on the computational methods for practical calculations, that brings together students from countries in Africa. The latest edition was scheduled to take place in Kigali, Rwanda, in June 2020 but had to be postponed.
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 Euros/year) matched by another 12'000 Euros/year by ICTP. This network funds "African researchers to visit other researchers or research groups in Africa for focused research collaboration for two months or more at a time and also support exchange of scientists between Africa and Europe for research collaborations and conference participation".

5.2.2 At the level of Master students

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). Of course, all went online.
Let us note, too, that Nicola Spaldin received the 2020 ETH "Golden Owl", an award given by the Association of students at ETH Zurich to lecturers who have provided exceptional teaching.

Developments

We tried to implement a coordinated semester class (MARVEL Academy, as described in the proposal for phase 2) made by different and separate modules in atomistic simulations, electronic structure simulations, multiscale methods, and machine learning. After discussion with EPFL, this was deemed to interfere too much with the semester-long classes, and so we are focusing more on the online activities and the education platform (see also the strategy for education in the pre-proposal for phase 3). In particular, Michele Ceriotti is preparing a MOOC on "Path integral methods for quantum thermodynamics and dynamics", supported by EPFL DRIL (Digital Resources for Instruction and Learning) fund and Giovanni Pizzi has just won such a DRIL support for "Jupyter web applications for quantum simulations".

5.2.3 For the younger generation

MARVEL high-school summer camp

In phase 2, MARVEL has initiated a summer camp for high school students, *Des atomes aux ordinateurs, à la découverte de la programmation scientifique*, where they could learn the basics of programming to study materials. With the support of the EPFL high-performance computing team SCITAS, and led by Michele Ceriotti, a team of six MARVEL volunteer postdocs and PhD students lead the students through a basic introduction to Python to applied exercises on topics such as the cellular automaton, molecular dynamics and machine learning.
The first edition in summer 2018 took place over 2 weeks and attracted 13 students — 4 women and 9 men. The 2019 edition was organized over a more compact single week and attracted 21 students — 10 women and 11 men. Both editions included visits to laboratories, and student evaluations were overwhelmingly positive: participants enjoyed attending the camp and were motivated to learn more about the topic.
A new edition planned on June 29 – July 3, 2020 had to be cancelled as no event was allowed on the EPFL campus at that time. A 2021 edition is tentatively set for this summer (June 28 – July 2, 2021). In all editions, half of the seats are reserved for young women.

Other activities

Usually MARVEL members participate in educational activities for the younger generation, in the classes or with lab visits, all kind of activities made impossible by the COVID-19 crisis. In 2017 in Fribourg and in 2019 in Porrentruy, MARVEL participated in thematic days organized by EPFL Education Outreach Department in high schools to allow students to discover various research domains within their own four walls, with conferences and feature demonstrations.

5.3 Equal opportunities

Following the year 4 site visit and the comments received afterwards from the SNSF research council, the equal opportunities strategy has been adapted, reallocating about 600 kCHF of budget to cover additional actions with the purpose of increasing the female presence within MARVEL. This is a continuation of the actions already planned in the initial strategy for phase 2. These efforts were recognized and highly appreciated by the review panel at the year 6 site visit and in the associated report. The review panel also acknowledged the sig-

nificant increase in the number of female PhD students.

5.3.1 Numbers

Increasing the proportion of women scientists within MARVEL is a challenge. At the national level, the proportion of women in MARVEL disciplines (physics, chemistry, materials science and computer science) is very low. For example, at EPFL, at the PhD level, the proportion of women is around 22% in physics and computer science and 35% in chemistry and materials science, with a very slight growth trend in recent years. The MARVEL numbers are similar, as can be seen in Table 5.1.
In year 7, the absolute number of women involved in MARVEL increased at the level of the group leaders. This was a consequence of the Agility Plus call, which brought four new female PIs to the NCCR and increased the share of women from 10 to 17%. The addition of one new female PhD student and a decrease of 9 in the number of male PhD students together led to an increase to 33% of women at the PhD level. The share of women at the postdoc level increased somewhat due to a decrease in the number of male postdocs. The total number of people at the senior researcher level over the years is too low for it to be possible to comment on the overall trend. The objective of phase 2 was to double the number of female PhD students within the NCCR, and with 19 in year 7 compared to 9 in year 3, we have already achieved this objective! Hopefully the increase in the number of women at the PhD level will lead to a similar increase at the postdoc level in the near future. However, this is not guaranteed as we know unfortunately that the pipeline is leaky. We need to think of ways to keep proportionally as many female PhD students as male in the academic world (e.g., betterscience.ch or slow scholarship initiatives).

5.3.2 Advancements of women scientists

Leadership of projects & allocation of funding

Following the call for new Agility Plus projects, a committee headed by Clémence Corminboeuf selected in early 2020 four new female PIs, one computational,

- Sereina Riniker, PATT at ETHZ, on "improving the generation and sampling of crystal packings with machine learning" and integrated in D&D1,

and three experimental,

- Ana Akrap, SNSF professor at UniFR, on "topological materials with intrinsic magnetic ordering" and integrated in D&D6,
- Emiliana Fabbri, senior researcher at PSI and 2020 PRIMA recipient, on the "search for MOF-based catalysts for the electrochemical splitting of water" and integrated in D&D4,
- Marta Gibert, SNSF professor at UZH, on the "electronic properties of $SrCrO_3$ thin films " and integrated in D&D5.

All four chose to use MARVEL money to pay a PhD student for two years. All have been already selected, two have started in 2020 and two will start in February and March 2021.

INSPIRE Potentials fellowships

Since the first call in spring 2016, we continue with two calls per year for female Master's students for the new MARVEL INSPIRE Potentials fellowship. Due to the COVID-19 crisis, the two recipients from the October 2019 call, Dune André at EPFL and Yuting Chen at Empa, had to switch online right after starting, which was not easy. Two of the three recipients from the April 2019 call had also to finish their work online. We wondered about the relevance of maintaining the 2020 calls and, indeed, the applicants were fewer. The main difference, though, was the greater number of "local" applicants, already studying in Swiss universities which are members of the MARVEL network. Three fellowships were awarded in spring 2020, to Veronica Michel (ETHZ) in the Spaldin group at ETHZ, Miriam Stuke (UniBas) in the von Lilienfeld group at UniBas and Maria Pakhnova (MIPT, Moscow) in the Ceriotti group at EPFL. In the latter case, the pandemic situation prevented Maria from coming to Switzerland. She is untertaking her Master's project completely remotely from Moscow and the amount of the fellowship was consequently reduced to 800 CHF per month. Two fellowships were awarded in autumn, to Elena Gazzarrini (King's College London) in the Marzari group at EPFL and Yuri Cho (UniBas) in the von Lilienfeld group at UniBas, who will start their projects in January and March 2021, respectively.
Due to the COVID-19 crisis and subsequent remote work, the feedback of the students is varied. Some were fully satisfied by the supervision and impressed by the online support and the personal engagement. For others, the experience helped them learn to be autonomous

	year 1		year 2		year 3		year 4		year 5		year 6		year 7	
	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%	6 17%	29 83%
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%	4 24%	13 76%
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%	9 18%	40 82%
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%	19 33%	38 67%

Table 5.1: *Number and share of women (W) and men (M) involved in MARVEL in years 1 to 7 (From NIRA).*

but was at the same time difficult: they required regular contact with the supervisor for the project to progress, and this was not always available. The MARVEL PIs have to integrate the fact that the students need close monitoring/mentoring, especially at the beginning of the project. Remote work amplified the differences between students, and shy students appear less proactive on Zoom and benefit less from the group dynamic.

In summary, since 2016, after 10 rounds and 64 applications, 31 fellows have been granted research projects in 13 different MARVEL groups in 6 institutions. Of these, 8 are already continuing at the PhD level in a MARVEL group or ex-MARVEL group. Of those who left, most (probably 10) are continuing at the PhD level abroad. In any case, these experiences are very useful, as they allow the recipient to discover the field of computational materials science and lead to the wish to pursue or not a PhD in this domain. For those continuing at the PhD level in this field, the INSPIRE Potentials project is often crucial in the decision to stay in this domain.

A constant difficulty, exacerbated by the COVID-19 crisis, is the low number of applicants. A quick survey of a few female PhD students coming from abroad revealed that, when asked if they considered doing a Master thesis abroad (i.e. outside the university which conferred their Bachelor's degree), they replied that they did not know this was possible or that they thought their institution would not have let them undertake a Master's in a different institution. As a consequence, they did not even search out such opportunities. While we encourage our Master's students to go abroad, these encouragements are clearly not general across Europe. We need to think about how to advertise the MARVEL INSPIRE Potentials fellowships and promote them more widely.

1 Career development

- We were planning to co-organize with the NCCR Digital Fabrication a new series of negotiation workshops for women in science with Nancy Houfek in October 2021. Due to the COVID-19 pandemic, the face-to-face workshops were cancelled. An online edition could not be organised due to other commitments on her part. We are now in the process of identifying and contacting other options, still in collaboration with the NCCR Digital Fabrication.
- MARVEL female researchers were regularly informed by email or through our internal newsletter of dedicated activities, mostly online, organized by EPFL or other participating institutions, and of existing offers in coaching or mentoring in MARVEL-related institutions. These are always advertised on our website.
- On March 5, 2020, as in the two previous years, the EPFL Alumni and Equal Opportunities offices organized their event for International Women's Day, the title for this year being "Shoot for the Moon". Again, MARVEL had a stand with information about its activities regarding equal opportunities. This was the last face-to-face event in which MARVEL was involved before the partial lockdown in Switzerland.

Recognition of female researchers' excellence and increase of their visibility

We continue to take care to promote the visibility of MARVEL women scientists, even if the opportunities were reduced in 2020.

Distinguished lectures and junior seminars After a break, the MARVEL distinguished lectures returned online (see Communication section). In this context, we are continuing to identify renowned female scientists for these lectures, with Silvia Picozzi (CNR-SPIN, Chieti, Italy)

presenting in December 2020 and Kristin Persson (Lawrence Berkeley Nat. Lab.) in April 2021 (postponed from spring 2020), out of the five distinguished lectures which took place in 2020 and are already planned for 2021. Since the beginning of MARVEL, 9 lectures out of 24 were given by women, and half of them (5 out of 10) since the beginning of phase 2.
An effort has been made to feature the diversity of MARVEL in the speakers presenting at the junior seminars, with 8 women and 16 men in the last 12 seminars.

Female Leadership in Science Based on an idea from Nicola Marzari, MARVEL's director, and sponsored by MARVEL, the EPFL Materials science and engineering department commissioned an art exhibit by Alban Kakulya, which unveiled in November 2018. The project was extended by the EPFL Equal Opportunities Office to "Female Leadership in Science", and portrayed 50 women professors at EPFL on the occasion of EPFL's 50^{th} anniversary. The project is continued with a "postcard edition" that will be sent to high schools and career guidance offices in western part of Switzerland. The portraits will also be integrated in an exhibition by the Historic Museum of Lausanne to illustrate advances of women's rights and place in society for the 50^{th} anniversary of women's right to vote in Switzerland. After these successful experiments and in view of the positive reactions of the public and the users of the campus, the idea of proposing a permanent work of art became obvious, to pay tribute not only to the professors currently on campus, but also to those who will come over the years. In this context, it is necessary to find a work that could grow with the new arrivals and that would portray something organic and alive, a kind of "Tree of Scientific Life" in the words of Nicola Marzari. This inspired Alban Kakulya's idea to create a green wall on which the cut-out portraits would be fixed, in a double message of ecology and promotion of women scientists. This project must still be evaluated by EPFL, in particular the new Vice Presidency for Responsible Transformation, and must find financial support, but MARVEL is happy to be a part of the adventure.

Cross-NCCR women's day campaign MARVEL is planing to participate in the Cross-NCCR women's day campaign, launched by NCCRs QSIT and Digital Fabrication, with the diffusion on social media of short videos of female 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 it", starting on March 8, 2021, International Women's Day, and ending on October 31, the anniversary of the first Swiss election in which women were allowed to vote.

Women's representation in events MARVEL always puts a lot of attention on women's representation in educational and public events organized by MARVEL or in which MARVEL participates, although this could not happen in 2020 due to the cancellation of all these events.

5.3.3 Raising gender awareness

Work climate and gender equality

A survey on work climate and gender equality within MARVEL was sent at the beginning of March 2020 to all members (including PIs, senior researchers, postdocs, PhD students, present INSPIRE Potentials Master's students and the management team). The survey aimed to assess the work and gender climate in the NCCR, work-life balance, harassment, the perception of equal opportunities and the involvement of MARVEL in this context, as well as to identify areas for improvement. We received 80 replies (52%), 57 from men (49% of the total number of men) and 23 from women (61%), i.e. 71% of the answers were from men and 29% were from women.
The outcomes were briefly presented at the online site visit in April 2020 and the review panel received a more detailed report. Its conclusion states that MARVEL has a good working climate as well as a good gender climate. However, even if about half the respondents (men and women) feel that the opportunities for career advancement are equal, 44% women and 28% men feel that it is more difficult for women to progress in their careers. Moreover, regarding work-life balance, respondents mostly feel that caring responsibilities are more of a disadvantage in women's careers than in men's careers. This feeling is again more pronounced for women than for men. In summary, within MARVEL the climate and feeling are good, but the perception of the equality in career advancement is less positive. This gives an indication of one field in which we should act. MARVEL is not immune to harassment. It is nevertheless encouraging to see that occurrences of harassment are rare. We note, however, that people should be better informed regarding where to get advice and how to proceed in case of harassment. Finally, one encouraging aspect is that almost everybody agrees that MARVEL's work on equal opportunities is relevant and half of respondents have become

Figure 3: *Action for girls in 2020. From left to right:* Coding club des filles*; summer camp* Matériaux super géniaux*;* Polythème *workshop on materials; chemistry summer camp (© EPFL SPS for all pictures).*

more aware of gender-bias concepts since joining MARVEL.
We are integrating the outcomes of the survey in the deployment of the strategy for equal opportunities in phase 3.

Gender-bias awareness training

We are convinced of the utmost importance of gender-bias awareness training and fully intend to continue these efforts. We took note of the suggestion of the review panel to integrate such an offer into other MARVEL activities, such as retreats or workshops. However, due to the COVID-19 crisis, no face-to-face events were organized. In the meantime, EPFL is preparing a mini-MOOC with Marianne Schmid Mast. It is organized in different modules as "Avoiding implicit bias", "Legal aspects & statistics", or "Avoiding implicit bias in recruitment procedures", and can therefore be adapted to different target groups (e.g., for student, without the module on recruitment). It should be ready in February 2021. We are considering using it within MARVEL, perhaps in combination with a short online workshop with Marianne Schmid Mast.
Since January 2021, a new Vice Presidency for Responsible Transformation at EPFL, led by Gisou van der Goot, former dean of the Faculty of Life Sciences, has been working to make the institution more inclusive and better able to respond to environmental and climate challenges. The Equal Opportunities office is attached to this new vice presidency and will enhance this type of offers.

5.3.4 Actions for girls, young women and future scientists

All the activities benefiting from MARVEL support were able to take place despite the COVID-19 pandemic. Significant effort has been made to maintain these activities. The scientific management staff has been reinforced, and some activities have been adapted and delivered online. Others were made possible by applying strict sanitary measures. Ongoing communication with parents was also one of the keys to the successful organisation of activities.

The sixth edition of the summer camp *Matériaux super géniaux*, August 17–21, welcomed 16 girls aged 11 to 13. The chemistry summer camp for girls and boys of the same age, August 10–14, could take place thanks to the respect of the sanitary rules: wearing of masks for adults, keeping distance, disinfecting, etc. Throughout both camps, participants made souvenir video sequences explaining the concepts studied. Intended for families, the videos replaced the in-person presentations at the end of the camp, which could not take place.

A first edition of the *Polythème* workshop *Diamant, alu, caoutchouc, ils sont fous ces matériaux !* took place face-to-face on September 2, 9 and 16, with 16 girls aged 7 to 10. A second edition, on November 25 and December 2, and a third one, on January 13 and 20, 2021, were given online. The girls were sent a kit of materials at home to enable them to carry out the experiments live, guided by the scientific mediators on Zoom. The January edition was split into two groups of 10, for comfort.

MARVEL continues its support of the mathematics workshops *Maths en jeu* and the coding workshops for girls *Coding club des filles*. In the spring, the mathematics workshops could not take place in the classroom and were instead continued through a series of videos sent to the participants together with email exchanges. In autumn, after a few sessions in the classroom, the workshops were adapted and delivered on Zoom. The satisfaction of the children and the very positive feedback from the parents testify to the success of the efforts in adaptating the workshops to an online format. To comply with the sanitary measures, the number of *Coding club des filles* workshops was doubled to ac-

commodate the same number of participants. In addition, it was possible to hold for the first time the workshops in German, in Bern.

Other actions

- One of the two SNSF Flexibility grants, which help to cover the external childcare costs for MARVEL parents, was used in 2018, renewed in 2019 and renewed for a second time in 2020.
- To keep an eye on developments in the field of equal opportunities, the MARVEL EO officer attended two online conferences in November 2020, the "NCCR MSE Conference on Equal Opportunity" on the 4^{th} and 5^{th}, and "Critical Gender and Diversity Knowledge. Challenges and Prospects" on the 20^{th} and 21^{st}. In particular, this gave the chance to discover such new initiatives as betterscience.ch and the slow scholarship movement, which favours a positive work-life balance.

5.4 Communication

5.4.1 Internal and external communication

Website and newsletter

We continued adding to the website (nccr-marvel.ch), contributing more than 25 news items on various activities, events, awards and other news of interest to the broader community. We also wrote 21 (as of January 21, 2021) feature stories and science highlights focused on the research of the groups. These go up to 56 since the beginning of phase 2. We published ten internal and scientific newsletters during the year. External readership of the scientific newsletter grew to 209 subscribers, up from 132 the year before and 63 two years before.

MARVEL distinguished lectures

MARVEL has organized distinguished lectures given by prominent experts in the fields covered by the NCCR. This is typically done on site at EPFL, giving the speaker the opportunity to deliver their presentation to the local community, and is 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 at www.materialscloud.org/learn). The speakers also have the opportunity to have discussions and meetings with local professors during their visit. As already reported, lectures organized on campus since the beginning of phase 2 were:

- Prof. Raffaele Resta (Democritos, IOM-CNR, Trieste, Italy), May 23, 2018.
- Prof. Sally Price (University College London, UK), September 6, 2018.
- Prof. Feliciano Giustino (Univ. Oxford, UK), December 5, 2018.
- Prof. Emily A. Carter (Princeton Univ.), June 17, 2019.
- Prof. Giulia Galli (Univ. Chicago), November 13, 2019. This MARVEL distinguished lecture was also an EPFL campus lecture.

As always, for equal opportunities reasons, a specific effort has been made to organize these events at 16:15, a time suitable for parents, for whom a late end might be problematic.
With the impossibility to hold in-person events in 2020, this has been suspended for most of the year, and we have then decided to continue the distinguished lecture series in videoconference 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, as well as a few private online-meetings with MARVEL PIs, which we organize, on or around the same day. Distinguished lectures held in this format are:

- Prof. Stefano Baroni (SISSA, Trieste, Italy), presented "Gauge invariance of heat and charge transport coefficients" on November 17, 2020, with more than 200 distinct connections, and about 170 attendees remaining throughout.
- Prof. Silvia Picozzi (Consiglio Nazionale delle Ricerche CNR-SPIN, Chieti, Italy) presented "Spin-orbit coupling: a small interaction leading to rich physics" on December 15, 2020, with more than 150 distinct connections, and about 125 attendees remaining throughout.
- Prof. Jens K. Nørskov (Technical Univ. Denmark) will present "Catalysis for sustainable production of fuels and chemicals" on February 18, 2021.
- Prof. Kristin Persson (Lawrence Berkeley National Laboratory) will present "The

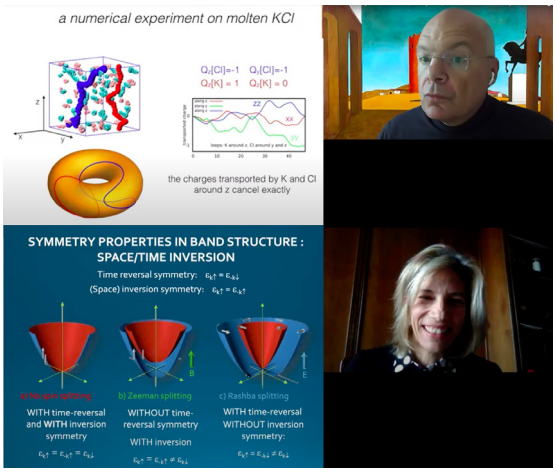

Figure 4: *Distinguished Lectures by Stefano Baroni (November 2020) and Silvia Picozzi (December 2020).*

Era of Data-Driven Materials Innovation and Design" on April 27, 2021.

- Prof. Georg Kresse (University of Vienna) on May 18, 2021.

5.4.2 Internal communication

Review and Retreats

The annual Review and Retreat, gathering all MARVEL members, group leaders as well as postdocs and students, takes place in September.
The fifth edition in 2018 (September 10–12) at EPFL was combined with the "International Workshop on Computational Design and Discovery of Novel Materials" (COMDI 2018).
The sixth edition took place at EPFL on September 5–6, 2019, with a total of 150 participants.
Due to the COVID-19 pandemic, the seventh Review and Retreat took place on September 10–11, 2020 as an online event, which created both a challenge and opportunity to vary the format, with more focus on junior researchers. In order to keep it interesting for everyone, the usual general project presentations delivered by the project leaders were replaced by sessions of 25 minutes per project which included three short presentations per project given by junior scientists on their research. The presentations were selected by the project leader, and covered important results/breakthroughs of the project that year. The presentations were strictly limited to 6 minutes. The rest of the time was devoted to Q&A and discussion. The program was held over two afternoons, which was necessary to accommodate Scientific Advisory Board (SAB) members living in the US who had up to 9 hours of time difference, and was also useful to keep sessions compact and interesting to follow. Ignoring short connections of less than 15 minutes, more than 180 distinct participants joined at least one of the two days, with 160 different attendees on the first day (and 120–140 connected at all times), and 134 on the second day (with 100–120 connected at all times). The event was followed by a meeting by the SAB, which then provided its feedback to the Executive Committee. In particular, the SAB enjoyed the new format offering a stronger focus on junior researchers and suggested involving them again more in future editions.

MARVEL junior seminars

MARVEL has been organizing regular junior seminars in order to strengthen interactions between the MARVEL junior scientists belonging to different research groups (i.e., PhD & postdocs either directly funded by the NCCR, or as a matching contribution). In year 5, MARVEL has held 9 junior seminars (every month except July, August, September) on campus at EPFL, and similarly in year 6, with 7 junior seminars. We interrupted the onsite events from March 2020 due to the COVID-19 pandemic. After a small break, we continued the junior seminars series in online format since May 2020, always on a monthly basis.
Each seminar consists of two 25-minute presentations, followed by time for discussion. In the pre-COVID 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 EPFL community interested in MARVEL research topics is welcome to attend, and does regularly. The organizing committee consists of delegates among PhD and postdoctoral students who act as chairs, with the mission to hold a lively Q&A session. The online version since May 2020 limits informal participants interactions and face-to-face discussions before and after the seminars. The remote meetings however have the very interesting advantage to make easier to have speakers from more distant locations (e.g. Zurich or Ticino), for whom it would otherwise be a little far to travel. Similarly, MARVEL members outside EPFL can much more easily assist. An effort is made to feature speakers that represent all research areas and all projects of MARVEL. In the last 12 junior seminars, 8 women and 16 men have presented their research.

Other meetings

All MARVEL projects meet regularly during the year, either in person or remotely.

5.4.3 External communication

Communicating MARVEL research

EurekAlert

We continued using EurekAlert and published 9 press releases on topics deemed to be of interest to the wider scientific and journalistic community. All were viewed more than 1000 times and 6 were viewed more than 2000 times, according to EurekAlert statistics. This is in line with our strategy of increased outreach to the wider scientific and journalist community.

Social media

Our social media work has focused on Twitter account @nccr_marvel, which had a following of 1'383 subscribers as of January 21, 2021, up from 929 at the end of the last reporting period. We posted an average of more than one Tweet/week over the year, earning more than 78'000 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 4.27%. According to 2018 industry benchmarks by Rival IQ, the median Twitter engagement rate across every industry is 0.046%.
We continue to manage an account on LinkedIn, primarily with the intention of building and reinforcing ties within the MARVEL community. This community is continuing to grow, particularly among researchers and students who have moved on and wish to keep in touch with the NCCR.

MARVEL in web news and in the press

The research of MARVEL teams has been covered in numerous press articles – in addition to being frequently featured on the MARVEL website and the websites of home institutions. For example, the EPFL news story "Atomistic modelling probes the behavior of matter at the center of Jupiter" on a result of Michele Ceriotti's group (September 2020) was featured in Science Daily, Decideo or SciTechDaily. The news story on "New experimental, theoretical evidence identifies jacutingaite as dual-topology insulator" on a result of Nicola Marzari's group was featured in Phys.org in March 2020.

Three minutes for my research

Presenting one's research in three minutes in plain language, to a non-specialist audience is a challenge met by five MARVEL PhD students at EPFL, three of them — Bardiya Valizadeh and Daniele Ongari, in Smit's group as well as Leonid Kahle in Marzari's group — selected for the EPFL final of "My Thesis in 180 Seconds" on March 7, 2019. This last year, Sauradeep Majundar in the Smit group participated in the FameLab competitions, with a similar challenge. On November 26 he was the Swiss representative in the online International Final 2020, which he won with a talk explaining how scientists are working to combat climate change by making new materials that can attract and capture carbon dioxide molecules

Events

Ig Nobel Award Tour Show

The Ig Nobel Prize is a satiric prize awarded annually to celebrate unusual achievements in scientific research. It honors "achievements that makes people laugh, and then think. The prizes are intended to celebrate the unusual, honor the imaginative — and spur people's interest in science, medicine, and technology." EPFL has welcomed four times the Ig Nobel Award Tour Show, with its creator Marc Abrahams and a line-up of Ig Nobel Prize winners, with the support of MARVEL. A great opportunity to see science from an original point of view, in a show that is both funny and inspiring, and an encouragement for scientists to think outside the box. In phase 2, we hosted the Ig Nobel Award Tour Show on March 25, 2019, with topics such as "Monitoring a brain cell of a locust while that locust watches selected highlights from the movie Star Wars" or "Can a cat be both a solid and a liquid?". On March 30, 2020, EPFL should have welcomed for the fifth time the Ig Nobel Award Tour Show, but the event was unfortunately canceled due to the COVID-19 pandemic. 2021 edition will not take place either for the same reason.

CECAM/MARVEL Mary Ann Mansigh conversation series

CECAM and MARVEL have initiated a new events series named "the Mary Ann Mansigh conversations", in honor to Mary Ann Mansigh Karlsen, a truly outstanding representa-

tive of the first generation of coders, whom we had welcomed at the EPFL in 2017. The goal is to provide the broad community with an opportunity to meet leading figures in domains in close proximity with the development and application of molecular and materials simulations. The guests engage in a conversation to describe expertise, approaches to research, and career paths in this area from a perspective not usually encountered in "standard" scientific presentations. In the first event, held at EPFL on May 8, 2019, Massimo Noro, formerly at Unilever and current Business Development Director at Daresbury labs, discussed with MARVEL PI William Curtin and with the audience the relevance of simulation for industry and his role as the leader of an important computing facility that interacts directly with industry. This conversation offered insight on how to promote and facilitate industrial use of simulation and modelling, and allowed the audience to meet a "living example" of a carrier path for simulators outside academia. Future events are planned, maybe early fall 2021, if on-site events are possible.

Other events

In 2020, all the events for the public at large were cancelled due to the COVID-19 crisis. In usual times, MARVEL takes all the opportunities to showcase its research, sharing and explaining it to the public. In phase 2, MARVEL presented at two occasions a stand with 3D movies and fun experiments to show how novel materials are created by computational design: at EPFL Scientastic, on 10 – 11 November 2018, and at the EPFL Open House part of the celebrations for its 50^{th} anniversary, on September 14–15, 2019.

6 Structural aspects

New associate professors

In September 2020, Michele Ceriotti and Oleg Yazyev, MARVEL PIs, Tenure Track Assistant Professors at EPFL, and part of the structural measures of phase 1, have been named Associate Professor of Materials Science in the School of Engineering and of Theoretical Physics in the School of Basic Sciences, respectively.
In addition, EPFL has made recent appointments that are very relevant to the MARVEL domain: Giuseppe Carleo, assistant professor of computational quantum science and Lenka Zdeborova, associate professor in statistical physics of computation. They will be involved in phase 3 activities.

Tenure-track position in computational materials science

The call for the promised tenure-track faculty position in computational materials science has been launched in August 2020 by the EPFL. Applications were invited covering research in any area of computational materials science, with a particular focus on computational and data-driven materials discovery. The position description stated that "examples of topics of interests include, but are not limited to, the development of theoretical and computational methods for materials modeling, and/or their application to understand, predict, design, and discover novel materials."
The search committee, chaired by MARVEL Director Nicola Marzari, is composed of 17 members, including 12 EPFL professors, 4 professors and senior researchers from outside EPFL, and one EPFL Master's student.
Following the December 14, 2020 deadline, 144 applications have been received (including 29 from women) and 11 applications have been shortlisted (including 4 women) for interviews scheduled between February 22 and March 5, 2021.

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.

Annex 2 Publications and published datasets lists

A. Publication list

All publications have been entered in NIRA, and are listed below. 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 since the beginning of phase 2 (May 2018 – January 2021).

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

1. All publications sorted by project

Project D&D1

Publications with peer review

⬢○ V. Rizzi, L. Bonati, N. Ansari, and M. Parrinello
The role of water in host-guest interaction
Nature Communications **12**, 93 (2021).
Group(s): Parrinello / Project(s): DD1

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

⬢○ M. Veit, D. M. Wilkins, Y. Yang, R. A. DiStasio, and M. Ceriotti
Predicting molecular dipole moments by combining atomic partial charges and atomic dipoles
The Journal of Chemical Physics **153**, 024113 (2020).
Group(s): Ceriotti / Project(s): DD1

○ G. Fraux, R. Cersonsky, and M. Ceriotti
Chemiscope: interactive structure-property explorer for materials and molecules
Journal of Open Source Software **5**, 2117 (2020).
Group(s): Ceriotti / Project(s): DD1

○ D. Mandelli, B. Hirshberg, and M. Parrinello
Metadynamics of Paths
Physical Review Letters **125**, 026001 (2020).
Group(s): Parrinello / Project(s): DD1

⬢○ N. Ansari, T. Karmakar, and M. Parrinello
Molecular Mechanism of Gas Solubility in Liquid: Constant Chemical Potential Molecular Dynamics Simulations
Journal of Chemical Theory and Computation **16**, 5279 (2020).
Group(s): Parrinello / Project(s): DD1

⬢○ K. Rossi, V. Jurásková, R. Wischert, L. Garel, C. Corminbœuf, and M. Ceriotti
Simulating Solvation and Acidity in Complex Mixtures with First-Principles Accuracy: The Case of CH_3SO_3H and H_2O_2 in Phenol

Journal of Chemical Theory and Computation **16**, 5139 (2020).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

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

B. Hirshberg, M. Invernizzi, and M. Parrinello
Path integral molecular dynamics for fermions: alleviating the sign problem with the Bogoliubov inequality
Chemical Physics **152**, 171102 (2020).
Group(s): Parrinello / Project(s): DD1

A. Fabrizio, R. Petraglia, and C. Corminboeuf
Balancing Density Functional Theory Interaction Energies in Charged Dimers Precursors to Organic Semiconductors
Journal of Chemical Theory and Computation **16**, 3530 (2020).
Group(s): Corminboeuf / Project(s): DD1

A. Fabrizio, B. Meyer, and C. Corminboeuf
Machine learning models of the energy curvature vs particle number for optimal tuning of long-range corrected functionals
The Journal of Chemical Physics **152**, 154103 (2020).
Group(s): Corminboeuf / Project(s): DD1

L. Bonati, V. Rizzi, and M. Parrinello
Data-Driven Collective Variables for Enhanced Sampling
The Journal of Physical Chemistry Letters **11**, 2998 (2020).
Group(s): Parrinello / Project(s): DD1

A. Fabrizio, K. R. Briling, A. Grisafi, and C. Corminboeuf
Learning (from) the Electron Density: Transferability, Conformational and Chemical Diversity
CHIMIA **74**, 232 (2020).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

J. A. Finkler and S. Goedecker
Funnel hopping Monte Carlo: An efficient method to overcome broken ergodicity
The Journal of Chemical Physics **152**, 164106 (2020).
Group(s): Goedecker / Project(s): DD1

D. Polino, E. Grifoni, R. Rousseau, and M. Parrinello
How Collective Phenomena Impact CO_2 Reactivity and Speciation in Different Media
The Journal of Physical Chemistry A **124**, 3963 (2020).
Group(s): Parrinello / Project(s): DD1

V. Kapil, D. M. Wilkins, J. Lan, and M. Ceriotti
Inexpensive modeling of quantum dynamics using path integral generalized Langevin equation thermostats
The Journal of Chemical Physics **152**, 124104 (2020).
Group(s): Ceriotti / Project(s): DD1

R. Fabregat, A. Fabrizio, B. Meyer, D. Hollas, and C. Corminboeuf
Hamiltonian-Reservoir Replica Exchange and Machine Learning Potentials for Computational Organic Chemistry
Journal of Chemical Theory and Computation **16**, 3084 (2020).
Group(s): Corminboeuf / Project(s): DD1

M. Invernizzi and M. Parrinello
Rethinking Metadynamics: from Bias Potentials to Probability Distributions
The Journal of Physical Chemistry Letters **11**, 2731 (2020).
Group(s): Parrinello / Project(s): DD1

A. Fabrizio, K. R. Briling, D. D. Girardier, and C. Corminboeuf
Learning on-top: regressing the on-top pair density for real-space visualization of electron correlation
The Journal of Chemical Physics **153**, 204111 (2020).
Group(s): Corminboeuf / Project(s): DD1

H. Niu, L. Bonati, P. M. Piaggi, and M. Parrinello
Ab initio phase diagram and nucleation of gallium
Nature Communications **11**, 2654 (2020).
Group(s): Parrinello / Project(s): DD1

M. Invernizzi, P. M. Piaggi, and M. Parrinello
A Unified Approach to Enhanced Sampling
Physical Review X **10**, 041034 (2020).
Group(s): Parrinello / Project(s): DD1

M. D. Wodrich, A. Fabrizio, B. Meyer, and C. Corminboeuf
Data-powered augmented volcano plots for homogeneous catalysis
Chemical Science **16**, 12070 (2020).
Group(s): Corminboeuf / Project(s): DD1

A. Grisafi, J. Nigam, and M. Ceriotti
Multi-scale approach for the prediction of atomic scale properties
Chemical Science (2020), doi:10.1039/D0SC04934D.
Group(s): Ceriotti / Project(s): DD1

B. Parsaeifard, D. S. De, A. S. Christensen, F. A. Faber, E. Kocer, S. De, J. Behler, A. von Lilienfeld, and S. Goedecker
An assessment of the structural resolution of various fingerprints commonly used in machine learning
Machine Learning: Science and Technology (2020), doi:10.1088/2632-2153/abb212.
Group(s): Goedecker, von Lilienfeld / Project(s): DD1, Inc2

M. Asgari, R. Semino, P. A. Schouwink, I. Kochetygov, J. Tarver, O. Trukhina, R. Krishna, C. M. Brown, M. Ceriotti, and W. L. Queen
Understanding How Ligand Functionalization Influences CO_2 and N_2 Adsorption in a Sodalite Metal-Organic Framework
Chemistry of Materials **32**, 1526 (2020).
Group(s): Ceriotti, Queen / Project(s): DD1, PP7

I. Errea, F. Belli, L. Monacelli, A. Sanna, T. Koretsune, T. Tadano, R. Bianco, M. Calandra, R. Arita, F. Mauri, and J. Flores-Livas
Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride
Nature **578**, 66 (2020).
Group(s): Goedecker / Project(s): DD1

G. Fisicaro, S. Filice, S. Scalese, G. Compagnini, R. Reitano, L. Genovese, S. Goedecker, I. Deretzis, and A. La Magna
Wet Environment Effects for Ethanol and Water Adsorption on Anatase TiO_2 (101) Surfaces
The Journal of Physical Chemistry C **124**, 2406 (2020).
Group(s): Goedecker / Project(s): DD1

J. A. Flores-Livas
Crystal structure prediction of magnetic materials
Journal of Physics: Condensed Matter **32**, 294002 (2020).
Group(s): Goedecker / Project(s): DD1

J. A. Flores-Livas, L. Boeri, A. Sanna, G. Profeta, R. Arita, and M. Eremets
A perspective on conventional high-temperature superconductors at high pressure: Methods and materials
Physics Reports **856**, 1 (2020).
Group(s): Goedecker / Project(s): DD1

F. Musil and M. Ceriotti
Machine Learning at the Atomic Scale
CHIMIA **73**, 972 (2019).
Group(s): Ceriotti / Project(s): DD1

A. Fabrizio, B. Meyer, R. Fabregat, and C. Corminboeuf
Quantum Chemistry Meets Machine Learning
CHIMIA **73**, 983 (2019).
Group(s): Corminboeuf / Project(s): DD1

A. Grisafi and M. Ceriotti
Incorporating long-range physics in atomic-scale machine learning
The Journal of Chemical Physics **151**, 204105 (2019).
Group(s): Ceriotti / Project(s): DD1

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

J. Zhang, Y. I. Yang, and F. Noé
Targeted Adversarial Learning Optimized Sampling
The Journal of Physical Chemistry Letters **10**, 5791 (2019).
Group(s): Parrinello / Project(s): DD1

B. A. Helfrecht, R. Semino, G. Pireddu, S. M. Auerbach, and M. Ceriotti
A new kind of atlas of zeolite building blocks
The Journal of Chemical Physics **151**, 154112 (2019).
Group(s): Ceriotti / Project(s): DD1

T. Karmakar, P. M. Piaggi, and M. Parrinello
Molecular Dynamics Simulations of Crystal Nucleation from Solution at Constant Chemical Potential
Journal of Chemical Theory and Computation **15**, 6923 (2019).
Group(s): Parrinello / Project(s): DD1

V. Kapil, E. Engel, M. Rossi, and M. Ceriotti
Assessment of Approximate Methods for Anharmonic Free Energies
Journal of Chemical Theory and Computation **15**, 5845 (2019).
Group(s): Ceriotti / Project(s): DD1

D. Dutta, D. S. De, D. Fan, S. Roy, G. Alfieri, M. Camarda, M. Amsler, J. Lehmann, H. Bartolf, S. Goedecker, and T. A. Jung
Evidence for carbon clusters present near thermal gate oxides affecting the electronic band structure in SiC-MOSFET
Applied Physics Letters **115**, 101601 (2019).
Group(s): Goedecker / Project(s): DD1

Y. Yang, K. U. Lao, D. M. Wilkins, A. Grisafi, M. Ceriotti, and R. A. DiStasio Jr.
Quantum mechanical static dipole polarizabilities in the QM7b and AlphaML showcase databases
Scientific Data **6**, 152 (2019).
Group(s): Ceriotti / Project(s): DD1

D. Han, T. Karmakar, Z. Bjelobrk, J. Gong, and M. Parrinello
Solvent-mediated morphology selection of the active pharmaceutical ingredient isoniazid: Experimental and simulation studies
Chemical Engineering Science **204**, 320 (2019).
Group(s): Parrinello / Project(s): DD1

L. Bonati, Y.-Y. Zhang, and M. Parrinello
Neural networks-based variationally enhanced sampling
Proceedings of the National Academy of Science of the USA **116**, 17641 (2019).
Group(s): Parrinello / Project(s): DD1

S. Faraji, S. A. Ghasemi, B. Parsaeifard, and S. Goedecker
Surface reconstructions and premelting of the (100) CaF_2 surface
Physical Chemistry Chemical Physics **21**, 16270 (2019).
Group(s): Goedecker / Project(s): DD1

P. M. Piaggi and M. Parrinello
Calculation of phase diagrams in the multithermal-multibaric ensemble
The Journal of Chemical Physics **150**, 244119 (2019).
Group(s): Parrinello / Project(s): DD1

H. Niu, Y. I. Yang, and M. Parrinello
Temperature Dependence of Homogeneous Nucleation in Ice
Physical Review Letters **122**, 245501 (2019).
Group(s): Parrinello / Project(s): DD1

S. Pérez-Conesa, P. M. Piaggi, and M. Parrinello
A local fingerprint for hydrophobicity and hydrophilicity: From methane to peptides
The Journal of Chemical Physics **150**, 204103 (2019).
Group(s): Parrinello / Project(s): DD1

M. Graužinytė, D. Tomerini, S. Goedecker, and J. A. Flores-Livas
A Divalent Path to Enhance p-Type Conductivity in a SnO Transparent Semiconductor
The Journal of Physical Chemistry C **123**, 14909 (2019).
Group(s): Goedecker / Project(s): DD1

Z. Bjelobrk, P. M. Piaggi, T. Weber, T. Karmakar, M. Mazzotti, and M. Parrinello
Naphthalene crystal shape prediction from molecular dynamics simulations
CrystEngComm **21**, 3280 (2019).
Group(s): Parrinello / Project(s): DD1

B. Meyer, S. Barthel, A. Mace, L. Vannay, B. Guillot, B. Smit, and C. Corminboeuf
DORI Reveals the Influence of Noncovalent Interactions on Covalent Bonding Patterns in Molecular Crystals Under Pressure
The Journal of Physical Chemistry Letters **10**, 1482 (2019).
Group(s): Corminboeuf, Smit / Project(s): DD1, DD4

M. J. Willatt, F. Musil, and M. Ceriotti
Atom-density representations for machine learning
The Journal of Chemical Physics **150**, 154110 (2019).
Group(s): Ceriotti / Project(s): DD1

R. A. Puglisi, S. Caccamo, C. Bongiorno, G. Fisicaro, L. Genovese, S. Goedecker, G. Mannino, and A. La Magna
Direct observation of single organic molecules grafted on the surface of a silicon nanowire
Scientific Reports **9**, 5647 (2019).
Group(s): Goedecker / Project(s): DD1

J. A. Flores-Livas, R. Sarmiento-Pérez, S. Botti, S. Goedecker, and M. A. L. Marques
Rare-earth magnetic nitride perovskites
JPhys Materials **2**, 025003 (2019).
Group(s): Goedecker / Project(s): DD1

M. Invernizzi and M. Parrinello
Making the best of a bad situation: a multiscale approach to free energy calculation
Journal of Chemical Theory and Computation **15**, 2187 (2019).
Group(s): Parrinello / Project(s): DD1

V. Kapil, M. Rossi, O. Marsalek, R. Petraglia, Y. Litman, T. Spura, B. Cheng,

A. Cuzzocrea, R. H. Meissner, D. M. Wilkins, B. A. Helfrecht, P. Juda, S. P. Bienvenue, W. Fang, J. Kessler, I. Poltavsky, S. Vandenbrande, J. Wieme, C. Corminboeuf, T. D. Kühne, D. E. Manolopoulos, T. E. Markland, J. O. Richardson, A. Tkatchenko, G. A. Tribello, V. V. Speybroeck, and M. Ceriotti
i-PI 2.0: A universal force engine for advanced molecular simulations

Computer Physics Communications **236**, 214 (2019).

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

O. Andreussi, N. G. Hörmann, F. Nattino, G. Fisicaro, S. Goedecker, and N. Marzari
Solvent-Aware Interfaces in Continuum Solvation

Journal of Chemical Theory and Computation **15**, 1996 (2019).

Group(s): Goedecker, Marzari / Project(s): DD1, DD3

P. M. Piaggi and M. Parrinello
Multithermal-multibaric molecular simulations from a variational principle

Physical Review Letters **122**, 050601 (2019).

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

J. Debnath, M. Invernizzi, and M. Parrinello
Enhanced sampling of transition states

Journal of Chemical Theory and Computation **15**, 2454 (2019).

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

M. Asgari, R. Semino, P. Schouwink, I. Kochetygov, O. Trukhina, J. D. Tarver, S. Bulut, S. Yang, C. M. Brown, M. Ceriotti, and W. L. Queen
An In-Situ Neutron Diffraction and DFT Study of Hydrogen Adsorption in a Sodalite-Type Metal-Organic Framework, Cu-BTTri

European Journal of Inorganic Chemistry **2019**, 1147 (2019).

Group(s): Ceriotti, Queen / Project(s): DD1, PP7

A. Grisafi, A. Fabrizio, B. Meyer, D. M. Wilkins, C. Corminboeuf, and M. Ceriotti
Transferable Machine-Learning Model of the Electron Density

ACS Central Science **5**, 57 (2019).

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

E. A. Engel, A. Anelli, A. Hofstetter, F. Paruzzo, L. Emsley, and M. Ceriotti
A Bayesian approach to NMR crystal structure determination

Physical Chemistry Chemical Physics **21**, 23385 (2019).

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

A. Fabrizio, A. Grisafi, B. Meyer, M. Ceriotti, and C. Corminboeuf
Electron density learning of non-covalent systems

Chemical Science **10**, 9424 (2019).

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

M. Graužinytė, S. Botti, M. A. L. Marques, S. Goedecker, and J. A. Flores-Livas
Computational acceleration of prospective dopant discovery in cuprous iodide

Physical Chemistry Chemical Physics **21**, 18839 (2019).

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

A. Grisafi, A. Fabrizio, B. Meyer, D. M. Wilkins, C. Corminboeuf, and M. Ceriotti
Transferable Machine-Learning Model of the Electron Density

ACS Central Science **5**, 57 (2019).

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

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).

Group(s): Ceriotti / Project(s): DD1, DD2

F. M. Paruzzo, A. Hofstetter, F. Musil, S. De, M. Ceriotti, and L. Emsley
Chemical shifts in molecular solids by machine learning

Nature Communications **9**, 4501 (2018).

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

M. Graužinytė, S. Goedecker, and J. A. Flores-Livas
Towards bipolar tin monoxide: Revealing unexplored dopants

Physical Review Materials **2**, 104604 (2018).

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

J. S. C. Kearney, M. Graužinytė, D. Smith, D. Sneed, C. Childs, J. Hinton, C. Park, J. S. Smith, E. Kim, S. D. S. Fitch, A. L. Hector, C. J. Pickard, J. A. Flores-Livas, and A. Salamat
Pressure-Tuneable Visible-Range Band Gap in the Ionic Spinel Tin Nitride

Angewandte Chemie International Edition **57**, 11623 (2018).

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

J. A. Flores-Livas, D. Tomerini, M. Amsler, A. Boziki, U. Rothlisberger, and S. Goedecker
Emergence of hidden phases of methylammonium lead iodide ($CH_3NH_3PbI_3$) upon compression
Physical Review Materials **2**, 085201 (2018).
Group(s): Goedecker, Röthlisberger / Project(s): DD1, VP2, HP4

E. Rucavado, M. Graužinytė, J. A. Flores-Livas, Q. Jeangros, F. Landucci, Y. Lee, T. Koida, S. Goedecker, A. Hessler-Wyser, C. Ballif, and M. Morales-Masis
New Route for "Cold-Passivation" of Defects in Tin-Based Oxides
The Journal of Physical Chemistry C **122**, 17612 (2018).
Group(s): Goedecker / Project(s): DD1

J. A. Flores-Livas, M. Graužinytė, L. Boeri, G. Profeta, and A. Sanna
Superconductivity in doped polyethylene at high pressure
The European Physical Journal B **91**, 176 (2018).
Group(s): Goedecker / Project(s): DD1

J. Yang, S. De, J. E. Campbell, S. Li, M. Ceriotti, and G. M. Day
Large-Scale Computational Screening of Molecular Organic Semiconductors Using Crystal Structure Prediction
Chemistry of Materials **30**, 4361 (2018).
Group(s): Ceriotti / Project(s): DD1

D. S. De, S. Saha, L. Genovese, and S. Goedecker
Influence of an external electric field on the potential-energy surface of alkali-metal-decorated C_{60}
Physical Review A **97**, 063401 (2018).
Group(s): Goedecker / Project(s): DD1

Y. I. Yang and M. Parrinello
Refining Collective Coordinates and Improving Free Energy Representation in Variational Enhanced Sampling
Journal of Chemical Theory and Computation **14**, 2889 (2018).
Group(s): Parrinello / Project(s): DD1

V. Kapil, A. Cuzzocrea, and M. Ceriotti
Anisotropy of the Proton Momentum Distribution in Water
The Journal of Physical Chemistry B **122**, 6048 (2018).
Group(s): Ceriotti / Project(s): DD1

L. Vannay, B. Meyer, R. Petraglia, G. Sforazzini, M. Ceriotti, and C. Corminboeuf
Analyzing Fluxional Molecules Using DORI
Journal of Chemical Theory and Computation **14**, 2370 (2018).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

L. E. Ratcliff, A. Degomme, J. A. Flores-Livas, S. Goedecker, and L. Genovese
Affordable and accurate large-scale hybrid-functional calculations on GPU-accelerated supercomputers
Journal of Physics: Condensed Matter **30**, 095901 (2018).
Group(s): Goedecker / Project(s): DD1

B. Meyer, B. Sawatlon, S. Heinen, O. A. von Lilienfeld, and C. Corminboeuf
Machine learning meets volcano plots: computational discovery of cross-coupling catalysts
Chemical Science **9**, 7069 (2018).
Group(s): Corminboeuf, von Lilienfeld / Project(s): DD1, Inc2

F. Musil, S. De, J. Yang, J. E. Campbell, G. M. Day, and M. Ceriotti
Machine learning for the structure-energy-property landscapes of molecular crystals
Chemical Science **9**, 1289 (2018).
Group(s): Ceriotti / Project(s): HP5, DD1

P. Gasparotto, R. H. Meissner, and M. Ceriotti
Recognizing Local and Global Structural Motifs at the Atomic Scale
Journal of Chemical Theory and Computation **14**, 486 (2018).
Group(s): Ceriotti / Project(s): DD1

D. Sankar De, J. A. Flores-Livas, S. Saha, L. Genovese, and S. Goedecker
Stable structures of exohedrally decorated C_{60}-fullerenes
Carbon **129**, 847 (2018).
Group(s): Goedecker / Project(s): HP4, DD1

P. M. Piaggi and M. Parrinello
Predicting polymorphism in molecular crystals using orientational entropy
Proceedings of the National Academy of Science of the USA **115**, 10251 (2018).
Group(s): Parrinello / Project(s): DD1

D. Mendels, J. McCarty, P. M. Piaggi, and M. Parrinello
Searching for Entropically Stabilized Phases: The Case of Silver Iodide
The Journal of Physical Chemistry C **122**, 1786

(2018).

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

- K. Tarak, P. M. Piaggi, C. Perego, and M. Parrinello
  A Cannibalistic Approach to Grand Canonical Crystal Growth
  Journal of Chemical Theory and Computation **14**, 2678 (2018).
  Group(s): Parrinello / Project(s): DD1

- H. Niu, P. M. Piaggi, M. Invernizzi, and M. Parrinello
  Molecular dynamics simulations of liquid silica crystallisation
  Proceedings of the National Academy of Science of the USA **115**, 5348 (2018).
  Group(s): Parrinello / Project(s): DD1

- Y. Wang, O. Valsson, P. Tiwary, M. Parrinello, and K. Lindorff-Larsen
  Frequency adaptive metadynamics for the calculation of rare-event kinetics
  The Journal of Chemical Physics **149**, 072309 (2018).
  Group(s): Parrinello / Project(s): DD1

- C. Perego, O. Valsson, and M. Parrinello
  Chemical potential calculations in non-homogeneous liquids
  The Journal of Chemical Physics **149**, 072305 (2018).
  Group(s): Parrinello / Project(s): DD1

- Y. I. Yang, H. Niu, and M. Parrinello
  Combining Metadynamics and Integrated Tempering Sampling
  The Journal of Physical Chemistry Letters **9**, 6426 (2018).
  Group(s): Parrinello / Project(s): DD1

- L. Bonati and M. Parrinello
  Silicon liquid structure and crystal nucleation from ab initio *deep metadynamics*
  Physical Review Letters **121**, 265701 (2018).
  Group(s): Parrinello / Project(s): DD1

- G. Gryn'ova, K.-H. Lin, and C. Corminboeuf
  Read between the Molecules: Computational Insights into Organic Semiconductors
  Journal of the American Chemical Society **140**, 16370 (2018).
  Group(s): Corminboeuf / Project(s): DD1

Publications without peer review

- T. Dornheim, M. Invernizzi, J. Vorberger, and B. Hirshberg
  Attenuating the fermion sign problem in path intergral Monte Carlo simulations using the Bogoliubov inequality and thermodynamic integration
  arXiv:2009.11036 (2020).
  Group(s): Parrinello / Project(s): DD1

- O. Valsson and M. Parrinello
  Variationally Enhanced Sampling
  in *Handbook of Materials Modeling : Methods: Theory and Modeling*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2018), pp. 1–14.
  Group(s): Parrinello / Project(s): DD1

Project D&D2

Publications with peer review

- B. Yin, S. Yoshida, N. Tsuji, and W. A. Curtin
  Yield strength and misfit volumes of NiCoCr and implications for short-range-order
  Nature Communications **11**, 2507 (2020).
  Group(s): Curtin / Project(s): DD2

- M. Stricker, B. Yin, E. Mak, and W. A. Curtin
  Machine learning for metallurgy II. A neural-network potential for magnesium
  Physical Review Materials **4**, 103602 (2020).
  Group(s): Curtin / Project(s): DD2

- J. Nigam, S. Pozdnyakov, and M. Ceriotti
  Recursive evaluation and iterative contraction of N-body equivariant features
  The Journal of Chemical Physics **153**, 121101 (2020).
  Group(s): Ceriotti / Project(s): DD2

- M. Zamani, G. Imbalzano, N. Tappy, D. T. L. Alexander, S. Martí-Sánchez, L. Ghisalberti, Q. M. Ramasse, M. Friedl, G. Tütüncüoglu, L. Francaviglia, S. Bienvenue, C. Hébert, J. Arbiol, M. Ceriotti, and A. F. i Morral
  3D Ordering at the Liquid-Solid Polar Interface of Nanowires
  Advanced Materials **32**, 2001030 (2020).
  Group(s): Ceriotti / Project(s): DD2

- Y. Hu, B. A. Szajewski, D. Rodney, and W. A. Curtin
  Atomistic dislocation core energies and calibration of non-singular discrete dislocation dynamics
  Modelling and Simulation in Materials Science and Engineering **28**, 015005 (2020).
  Group(s): Curtin / Project(s): DD2

D. Marchand, A. Jain, A. Glensk, and W. A. Curtin
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Group(s): Shi, Yazyev / Project(s): PP7, DD6

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

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

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Physical Chemistry Chemical Physics **20**, 29661 (2018).

Group(s): Ceriotti / Project(s): DD1, DD2

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The Journal of Physical Chemistry Letters **9**, 1880 (2018).

Group(s): Pasquarello / Project(s): VP2, DD3, DD4

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ACS Catalysis **8**, 5847 (2018).

Group(s): Pasquarello / Project(s): VP2, DD3, DD4

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Chemistry of Materials **30**, 94 (2018).

Group(s): Pasquarello / Project(s): VP2, DD3, DD4

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

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

G. Prandini, A. Marrazzo, I. E. Castelli, N. Mounet, and N. Marzari

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

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

Phase 2 PIs

Group of Ulrich Aschauer

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Physical Review Research **2**, 042040 (2020).
Group(s): Aschauer / Project(s): DD5

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Physical Review Research **2**, 023313 (2020).
Group(s): Aschauer, Marzari / Project(s): DD5, DD3

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Physical Review B **99**, 094102 (2019).
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Physical Review Letters **121**, 055701 (2018).
Group(s): Aschauer, Staub / Project(s): PP7, DD5

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Surface and Defect Chemistry of Oxide Materials
CHIMIA **72**, 286 (2018).
Group(s): Aschauer / Project(s): DD5

Group of Michele Ceriotti

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Nature **589**, 59 (2021).
Group(s): Ceriotti / Project(s): DD1

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The Journal of Chemical Physics **153**, 121101 (2020).
Group(s): Ceriotti / Project(s): DD2

M. Zamani, G. Imbalzano, N. Tappy, D. T. L. Alexander, S. Martí-Sánchez, L. Ghisalberti, Q. M. Ramasse, M. Friedl, G. Tütüncüoglu, L. Francaviglia, S. Bienvenue, C. Hébert, J. Arbiol, M. Ceriotti, and A. F. i Morral
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Advanced Materials **32**, 2001030 (2020).
Group(s): Ceriotti / Project(s): DD2

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The Journal of Chemical Physics **153**, 024113 (2020).
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Journal of Open Source Software **5**, 2117 (2020).
Group(s): Ceriotti / Project(s): DD1

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Journal of Chemical Theory and Computation **16**, 5139 (2020).
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Chemistry of Materials **32**, 1526 (2020).
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CHIMIA **73**, 972 (2019).
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Journal of Chemical Theory and Computation **15**, 5845 (2019).
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International Journal of Quantum Chemistry **119**, e25872 (2019).
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The Journal of Chemical Physics **150**, 154110 (2019).
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Frontiers in Materials **6**, 53 (2019).
Group(s): Ceriotti / Project(s): DD2

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

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European Journal of Inorganic Chemistry **2019**, 1147 (2019).
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Transferable Machine-Learning Model of the Electron Density
ACS Central Science **5**, 57 (2019).
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Physical Chemistry Chemical Physics **21**, 23385 (2019).
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Chemical Science **10**, 9424 (2019).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

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Journal of Chemical Theory and Computation **15**, 906 (2019).
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Nature Communications **9**, 4501 (2018).
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Chemistry of Materials **30**, 4361 (2018).
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The Journal of Physical Chemistry B **122**, 6048 (2018).
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Journal of Chemical Theory and Computation **14**, 2370 (2018).
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Chemical Science **9**, 1289 (2018).
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Journal of Chemical Theory and Computation **14**, 486 (2018).
Group(s): Ceriotti / Project(s): DD1

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Simulating Solvation and Acidity in Complex Mixtures with First-Principles Accuracy: The Case of CH_3SO_3H and H_2O_2 in Phenol
Journal of Chemical Theory and Computation **16**, 5139 (2020).
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Journal of Chemical Theory and Computation **16**, 3530 (2020).
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The Journal of Chemical Physics **152**, 154103 (2020).
Group(s): Corminboeuf / Project(s): DD1

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Learning (from) the Electron Density: Transferability, Conformational and Chemical Diversity
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R. Fabregat, A. Fabrizio, B. Meyer, D. Hollas, and C. Corminboeuf
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Journal of Chemical Theory and Computation **16**, 3084 (2020).
Group(s): Corminboeuf / Project(s): DD1

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The Journal of Chemical Physics **153**, 204111 (2020).
Group(s): Corminboeuf / Project(s): DD1

M. D. Wodrich, A. Fabrizio, B. Meyer, and C. Corminboeuf
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Chemical Science **16**, 12070 (2020).
Group(s): Corminboeuf / Project(s): DD1

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Physical Chemistry Chemical Physics **22**, 19512 (2020).
Group(s): Corminboeuf, Smit, Tavernelli / Project(s): DD4

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CHIMIA **73**, 983 (2019).
Group(s): Corminboeuf / Project(s): DD1

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ChemCatChem **11**, 4096 (2019).
Group(s): Corminboeuf / Project(s): VP2

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The Journal of Physical Chemistry Letters **10**, 4259 (2019).
Group(s): Buonsanti, Corminboeuf / Project(s): VP2, PP7

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Journal of the American Chemical Society **141**, 12011 (2019).
Group(s): Corminboeuf, Fasel, Passerone / Project(s): DD3

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Computer Physics Communications **236**, 214 (2019).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

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ACS Central Science **5**, 558 (2019).
Group(s): Corminboeuf / Project(s): VP2

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Transferable Machine-Learning Model of the Electron Density
ACS Central Science **5**, 57 (2019).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

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Journal of Chemical Theory and Computation **14**, 2370 (2018).
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ChemCatChem **10**, 1592 (2018).
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Nature Communications **11**, 2131 (2020).

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

G. Smolentsev, M. A. Soldatov, B. Probst, C. Bachmann, N. Azzaroli, R. Alberto, M. Nachtegaal, and J. A. van Bokhoven

Structure of the Co^I Intermediate of a Cobalt Pentapyridyl Catalyst for Hydrogen Evolution Revealed by Time-Resolved X-ray Spectroscopy

ChemSusChem **11**, 3087 (2018).

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

G. Smolentsev, K. M. van Vliet, N. Azzaroli, J. A. van Bokhoven, A. M. Brouwer, B. de Bruin, M. Nachtegaal, and M. Tromp

Pump-probe XAS investigation of the triplet state of an Ir photosensitizer with chromenopyridinone ligands

Photochemical & Photobiological Sciences **17**, 896 (2018).

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

Group of Matthias Troyer

G. Pizzi, V. Vitale, R. Arita, S. Blügel, F. Freimuth, G. Géranton, M. Gibertini, D. Gresch, C. Johnson, T. Koretsune, J. Ibañez-Azpiroz, H. Lee, J.-M. Lihm, D. Marchand, A. Marrazzo, Y. Mokrousov, J. I. Mustafa, Y. Nohara, Y. Nomura, L. Paulatto, S. Poncé, T. Ponweiser, J. Qiao, F. Thöle, S. S. Tsirkin, M. Wierzbowska, N. Marzari, D. Vanderbilt, I. Souza, A. A. Mostofi, and J. R. Yates

Wannier90 as a community code: new features and applications

Journal of Physics: Condensed Matter **32**, 165902 (2020).

Group(s): Curtin, Marzari, Pizzi, Spaldin, Troyer, Yazyev / Project(s): OSP, PP6

G. Torlai, G. Mazzola, J. Carrasquilla, M. Troyer, R. Melko, and G. Carleo

Neural-network quantum state tomography

Nature Physics **14**, 447 (2018).

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

Q. Wu, S. Zhang, H.-F. Song, M. Troyer, and A. A. Soluyanov

WannierTools: An open-source software package for novel topological materials

Computer Physics Communications **224**, 405 (2018), http://www.wanniertools.com.

Group(s): Soluyanov, Troyer / Project(s): VP1, DD6

X. Feng, C. Yue, Z. Song, Q. Wu, and B. Wen

Topological Dirac nodal-net fermions in AlB_2-type TiB_2 and ZrB_2

Physical Review Materials **2**, 014202 (2018).

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

G. Mazzola, R. Helled, and S. Sorella

Phase Diagram of Hydrogen and a Hydrogen-Helium Mixture at Planetary Conditions by Quantum Monte Carlo Simulations

Physical Review Letters **120**, 025701 (2018).
Group(s): Troyer / Project(s): VP1

A. Scaramucci, H. Shinaoka, M. V. Mostovoy, M. Müller, C. Mudry, M. Troyer, and N. A. Spaldin
Multiferroic Magnetic Spirals Induced by Random Magnetic Exchanges
Physical Review X **8**, 011005 (2018).
Group(s): Spaldin, Troyer / Project(s): VP1

Q. Wu, C. Piveteau, Z. Song, and O. V. Yazyev
$MgTa_2N_3$: A reference Dirac semimetal
Physical Review B **98**, 081115(R) (2018).
Group(s): Troyer, Yazyev / Project(s): DD6

Group of Dirk van der Marel

Q. N. Meier, A. Stucky, J. Teyssier, S. M. Griffin, D. van der Marel, and N. A. Spaldin
Manifestation of structural Higgs and Goldstone modes in the hexagonal manganites
Physical Review B **102**, 014102 (2020).
Group(s): Spaldin, van der Marel / Project(s): VP1, PP7

MARVEL visitors

François Gygi (UC Davis)

M. D. LaCount and F. Gygi
Ensemble first-principles molecular dynamics simulations of water using the SCAN meta-GGA density functional
The Journal of Chemical Physics **151**, 164101 (2019).
Group(s): NCCR / Project(s): NCCR

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

Group of Clémence Corminboeuf

F. Song, M. Busch, B. Lassalle-Kaiser, C.-S. Hsu, E. Petkucheva, M. Bensimon, H. M. Chen, C. Corminboeuf, and X. Hu
A Bifunctional Iron Nickel Catalyst for the Oxygen Evolution Reaction
ChemRxiv. Preprint (2018), doi:10.26434/chemrxiv.7246859.
Group(s): Corminboeuf / Project(s): VP2

Group of Jürg Hutter

T. Duignan, G. K. Schenter, J. Fulton, T. Huthwelker, M. Balasubramanian, M. Galib, M. D. Baer, J. Wilhelm, J. Hutter, M. D. Ben, X. S. Zhao, and C. J. Mundy
Quantifying the hydration structure of sodium and potassium ions: taking additional steps on Jacob's Ladder
ChemRxiv. Preprint (2019), doi:10.26434/chemrxiv.7466426.v2.
Group(s): Hutter / Project(s): HP3

J. Hutter, J. Wilhelm, V. V. Rybkin, M. D. Ben, and J. VandeVondele
MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling
in *Handbook of Materials Modeling : Methods: Theory and Modeling*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2018), pp. 1–21.
Group(s): Hutter / Project(s): HP3

Group of Teodoro Laino

G. Materzanini, L. Kahle, A. Marcolongo, and N. Marzari
Electrolytes for Li-ion all-solid-state batteries: a first-principles comparative study of $Li_{10}GeP_2O_{12}$ and $Li_{10}GeP_2S_{12}$ in the LISICON and LGPS phases
arXiv:2010.08068 (2020).
Group(s): Laino, Marzari / Project(s): Inc1

Group of Mathieu Luisier

Á. Szabó, C. Klinkert, D. Campi, C. Stieger, N. Marzari, and M. Luisier
Ab initio simulation of band-to-band tunneling FETs with single- and few-layer 2-D materials as channels
arXiv:2012.04629 (2020).
Group(s): Marzari, Luisier / Project(s): DD3

Group of Nicola Marzari

G. Materzanini, L. Kahle, A. Marcolongo, and N. Marzari
Electrolytes for Li-ion all-solid-state batteries: a first-principles comparative study of $Li_{10}GeP_2O_{12}$ and $Li_{10}GeP_2S_{12}$ in the LISICON and LGPS phases
arXiv:2010.08068 (2020).
Group(s): Laino, Marzari / Project(s): Inc1

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
arXiv:2012.14751 (2020).
Group(s): Marzari / Project(s): DD3

I. Timrov, N. Marzari, and M. Cococcioni
Self-consistent Hubbard parameters from density-functional perturbation theory in the ultrasoft and projector-augmented wave formulations
arXiv:2011.03271, *to be published in* Physical Review B (2020).
Group(s): Marzari / Project(s): OSP

L. Banszerus, T. Sohier, A. Epping, F. Winkler, F. Libisch, F. Haupt, K. Watanabe, T. Taniguchi, K. Müller-Caspary, N. Marzari, F. Mauri, B. Beschoten, and C. Stampfer
Extraordinary high room-temperature carrier mobility in graphene-WSe_2 heterostructures
arXiv:1909.09523 (2019).
Group(s): Marzari / Project(s): DD3

N. Marzari
Materials Informatics: Overview
in *Handbook of Materials Modeling : Methods: Theory and Modeling*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2019), pp. 1–7.
Group(s): Marzari / Project(s): OSP

A. Cepellotti and N. Marzari
On the Kinetic Theory of Thermal Transport in Crystals
in *Handbook of Materials Modeling: Applications: Current and Emerging Materials*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2018), pp. 1–42.
Group(s): Marzari / Project(s): DD3

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

Ab initio simulation of band-to-band tunneling FETs with single- and few-layer 2-D materials as channels

arXiv:2012.04629 (2020).

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

G. Pizzi, S. Milana, A. C. Ferrari, N. Marzari, and M. Gibertini

Shear and breathing modes of layered materials

arXiv:2011.14681 (2020).

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

M. Uhrin, G. Pizzi, N. Mounet, N. Marzari, and P. Villars

A High-Throughput Computational Study Driven by the AiiDA Materials Informatics Framework and the PAULING FILE *as Reference Database*

in *Materials Informatics: Methods, Tools and Applications*, O. Isayev, A. Tropsha, and S. Curtarolo, eds. (John Wiley & Sons, Ltd, 2019), pp. 149–170.

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

Group of Titus Neupert

M. Iraola, J. L. Manes, B. Bradlyn, T. Neupert, M. G. Vergniory, and S. S. Tsirkin

IrRep: symmetry eigenvalues and irreducible representations of ab initio band structures

arXiv:2009.01764 (2020), http://irrep.dipc.org.

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

A. Nelson, T. Neupert, T. Bzdušek, and A. Alexandradinata

Multicellularity of delicate topological insulators

arXiv:2009.01863 (2020).

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

Group of Michele Parrinello

T. Dornheim, M. Invernizzi, J. Vorberger, and B. Hirshberg

Attenuating the fermion sign problem in path intergral Monte Carlo simulations using the Bogoliubov inequality and thermodynamic integration

arXiv:2009.11036 (2020).

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

O. Valsson and M. Parrinello

Variationally Enhanced Sampling

in *Handbook of Materials Modeling : Methods: Theory and Modeling*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2018), pp. 1–14.

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

Group of Daniele Passerone

L. Talirz and C. A. Pignedoli

Electronic Structure of Atomically Precise Graphene Nanoribbons

in *Handbook of Materials Modeling: Applications: Current and Emerging Materials*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2018), pp. 1–35.

Group(s): Passerone, Smit / Project(s): DD3, DD4

Group of Giovanni Pizzi

G. Pizzi, S. Milana, A. C. Ferrari, N. Marzari, and M. Gibertini

Shear and breathing modes of layered materials

arXiv:2011.14681 (2020).

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

M. Uhrin, G. Pizzi, N. Mounet, N. Marzari, and P. Villars

A High-Throughput Computational Study Driven by the AiiDA Materials Informatics Framework and the PAULING FILE *as Reference Database*

in *Materials Informatics: Methods, Tools and Applications*, O. Isayev, A. Tropsha, and S. Curtarolo, eds. (John Wiley & Sons, Ltd, 2019), pp. 149–170.

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

G. Pizzi, A. Togo, and B. Kozinsky

Provenance, workflows, and crystallographic tools in materials science: AiiDA, spglib, and seekpath

MRS Bulletin **43**, 696 (2018).

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

G. Pizzi

Open-Science Platform for Computational Materials Science: AiiDA and the Materials Cloud

in *Handbook of Materials Modeling : Methods: Theory and Modeling*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2018), pp. 1–24.

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

Group of Volker Roth

V. Nesterov, M. Wieser, and V. Roth

3DMolNet: A Generative Network for Molecular Structures

arXiv:2010.06477 (2020).

Group(s): Roth / Project(s): Inc2

Group of Ming Shi

M. Yao, H. Lee, N. Xu, Y. Wang, J. Ma, O. V. Yazyev, Y. Xiong, M. Shi, G. Aeppli, and Y. Soh
Switchable Weyl nodes in topological Kagome ferromagnet Fe_3Sn_2
arXiv:1810.01514 (2018).
Group(s): Shi, Yazyev / Project(s): DD6

Group of Berend Smit

K. M. Jablonka, S. M. Moosavi, M. Asgari, C. Ireland, L. Patiny, and B. Smit
A Data-Driven Perspective on the Colours of Metal-Organic Frameworks
ChemRxiv. Preprint. (2020), doi:10.26434/chemrxiv.13033217.v1.
Group(s): Smit / Project(s): DD4

L. Talirz and C. A. Pignedoli
Electronic Structure of Atomically Precise Graphene Nanoribbons
in *Handbook of Materials Modeling: Applications: Current and Emerging Materials*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2018), pp. 1–35.
Group(s): Passerone, Smit / Project(s): DD3, DD4

Group of Urs Staub

H. Ueda, M. Porer, J. R. L. Mardegan, S. Parchenko, N. Gurung, F. Fabrizi, M. Ramakrishnan, L. Boie, M. J. Neugebauer, B. Burganov, M. Burian, S. L. Johnson, K. Rossnagel, and U. Staub
Correlation between electronic and structural orders in 1T-$TiSe_2$
arXiv:2006.08983 (2020).
Group(s): Staub / Project(s): PP7

Group of Anatole von Lilienfeld

M. Schwilk, D. N. Tahchieva, and O. A. von Lilienfeld
Large yet bounded: Spin gap ranges in carbenes
arXiv:2004.10600 (2020).
Group(s): von Lilienfeld / Project(s): Inc2

B. Huang and O. A. von Lilienfeld
Dictionary of 140k GDB and ZINC derived AMONs
arXiv:2008.05260 (2020).
Group(s): von Lilienfeld / Project(s): Inc2

G. F. von Rudorff and O. A. von Lilienfeld
Solving the inverse materials design problem with alchemical chirality
arXiv:2008.02784 (2020).
Group(s): von Lilienfeld / Project(s): Inc2

B. Huang and O. A. von Lilienfeld
Ab initio machine learning in chemical compound space
arXiv:2012.07502 (2020).
Group(s): von Lilienfeld / Project(s): Inc2

F. A. Faber and O. A. von Lilienfeld
Modeling Materials Quantum Properties with Machine Learning
in *Materials Informatics: Methods, Tools and Applications*, O. Isayev, A. Tropsha, and S. Curtarolo, eds. (John Wiley & Sons, Ltd, 2019), pp. 171–179.
Group(s): von Lilienfeld / Project(s): Inc2

B. Huang, N. O. Symonds, and O. A. von Lilienfeld
Quantum Machine Learning in Chemistry and Materials
in *Handbook of Materials Modeling : Methods: Theory and Modeling*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2018), pp. 1–27.
Group(s): von Lilienfeld / Project(s): Inc2

Group of Oleg Yazyev

Q. Wu, J. Liu, and O. V. Yazyev
Landau Levels as a Probe for Band Topology in Graphene Moiré Superlattices
arXiv:2005.10620 (2020).
Group(s): Yazyev / Project(s): DD6

M. Yao, H. Lee, N. Xu, Y. Wang, J. Ma, O. V. Yazyev, Y. Xiong, M. Shi, G. Aeppli, and Y. Soh
Switchable Weyl nodes in topological Kagome ferromagnet Fe_3Sn_2
arXiv:1810.01514 (2018).
Group(s): Shi, Yazyev / Project(s): DD6

H. Lee and O. V. Yazyev
Plethora of Coexisting Topological Band Degeneracies in Nonsymmorphic Molecular Crystal $OsOF_5$
arXiv:1808.06346 (2018).
Group(s): Yazyev / Project(s): DD6

O. V. Yazyev
Modeling Disordered and Nanostructured Graphene
in *Handbook of Materials Modeling: Applications: Current and Emerging Materials*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2018), pp. 1–20.
Group(s): Yazyev / Project(s): DD6

B. Published datasets list

All published datasets resulting from MARVEL research are listed below, sorted by projects. It is also available on the dataset index page (nccr-marvel.ch/publications/dataset-index) on MARVEL website. Most of the datasets are available on the Materials Cloud *Archive* open repository.
We list datasets either resulting directly from the NCCR (marked with a red hexagon ⬢) or with minor contributions from the NCCR. All datasets are accessible in Open Access (OA). The following list cover the period since the beginning of phase 2 (May 2018 – January 2021).

Project D&D1

10.5281/zenodo.4174139
Research data for "Origins of structural and electronic transitions in disordered silicon", V. L. Deringer, N. Bernstein, G. Csányi, C. B. Mahmoud, M. Ceriotti, M. Wilson, D. A. Drabold, and S. R. Elliott

Related MARVEL publication

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

⬢ **10.24435/materialscloud:z9-zr**
Simulating solvation and acidity in complex mixtures with first-principles accuracy: the case of CH_3SO_3H and H_2O_2 in phenol, K. Rossi, V. Juraskova, R. Wischert, L. Garel, C. Corminboeuf, and M. Ceriotti

Related MARVEL publication

K. Rossi, V. Jurásková, R. Wischert, L. Garel, C. Corminbœuf, and M. Ceriotti
Simulating Solvation and Acidity in Complex Mixtures with First-Principles Accuracy: The Case of CH_3SO_3H and H_2O_2 in Phenol
Journal of Chemical Theory and Computation **16**, 5139 (2020).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

⬢ **10.24435/materialscloud:tr-t9**
Multi-scale approach for the prediction of atomic scale properties, A. Grisafi, J. Nigam, and M. Ceriotti

Related MARVEL publication

A. Grisafi, J. Nigam, and M. Ceriotti
Multi-scale approach for the prediction of atomic scale properties
Chemical Science (2020), doi:10.1039/D0SC04934D.
Group(s): Ceriotti / Project(s): DD1

⬢ **10.24435/materialscloud:s0-yx**
Data-powered augmented volcano plots for homogeneous catalysis, M. D. Wodrich, A. Fabrizio, B. Meyer, and C. Corminboeuf

Related MARVEL publications

A. Fabrizio, K. R. Briling, A. Grisafi, and C. Corminboeuf
Learning (from) the Electron Density: Transferability, Conformational and Chemical Diversity
CHIMIA **74**, 232 (2020).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

M. D. Wodrich, A. Fabrizio, B. Meyer, and C. Corminboeuf
Data-powered augmented volcano plots for homogeneous catalysis
Chemical Science **16**, 12070 (2020).
Group(s): Corminboeuf / Project(s): DD1

⬢ **10.24435/materialscloud:p3-1x**
The role of water in host-guest interaction, V. Rizzi, L. Bonati, N. Ansari, and M. Parrinello

Related MARVEL publication

V. Rizzi, L. Bonati, N. Ansari, and M. Parrinello
The role of water in host-guest interaction
Nature Communications **12**, 93 (2021).
Group(s): Parrinello / Project(s): DD1

⬢ **10.24435/materialscloud:k5-t2**
Molecular mechanism of gas solubility in liquid: constant chemical potential molecular dynamics simulations, N. Ansari, T. Karmakar, and M. Parrinello

Related MARVEL publication

N. Ansari, T. Karmakar, and M. Parrinello
Molecular Mechanism of Gas Solubility in Liquid: Constant Chemical Potential Molecular Dynamics Simulations
Journal of Chemical Theory and Computation **16**, 5279 (2020).
Group(s): Parrinello / Project(s): DD1

⬢ **10.24435/materialscloud:gr-w3**
A unified approach to enhanced sampling, M. Invernizzi, P. M. Piaggi, and M. Parrinello

Related MARVEL publication

M. Invernizzi, P. M. Piaggi, and M. Parrinello
A Unified Approach to Enhanced Sampling
Physical Review X **10**, 041034 (2020).
Group(s): Parrinello / Project(s): DD1

- **10.24435/materialscloud:8z-2p**
  Learning on-top: regressing the on-top pair density for real-space visualization of electron correlation, A. Fabrizio, K. R. Briling, D. D. Girardier, and C. Corminboeuf

  Related MARVEL publication

  A. Fabrizio, K. R. Briling, D. D. Girardier, and C. Corminboeuf
  Learning on-top: regressing the on-top pair density for real-space visualization of electron correlation

  The Journal of Chemical Physics **153**, 204111 (2020).

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

- **10.24435/materialscloud:2k-3h**
  Quantum mechanical dipole moments in the QM7b, 21k molecules of QM9, and MuML showcase datasets, M. Veit, D. M. Wilkins, Y. Yang, R. A. DiStasio Jr., and M. Ceriotti

  Related MARVEL publication

  M. Veit, D. M. Wilkins, Y. Yang, R. A. DiStasio, and M. Ceriotti
  Predicting molecular dipole moments by combining atomic partial charges and atomic dipoles

  The Journal of Chemical Physics **153**, 024113 (2020).

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

- **10.24435/materialscloud:2020.0039/v1**
  Ab-initio phase diagram and nucleation of gallium, H. Niu, L. Bonati, P. M. Piaggi, and M. Parrinello

  Related MARVEL publication

  H. Niu, L. Bonati, P. M. Piaggi, and M. Parrinello
  Ab initio phase diagram and nucleation of gallium

  Nature Communications **11**, 2654 (2020).

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

- **10.24435/materialscloud:2020.0035/v1**
  Data-Driven Collective Variables for Enhanced Sampling, L. Bonati, V. Rizzi, and M. Parrinello

  Related MARVEL publication

  L. Bonati, V. Rizzi, and M. Parrinello
  Data-Driven Collective Variables for Enhanced Sampling

  The Journal of Physical Chemistry Letters **11**, 2998 (2020).

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

- **10.24435/materialscloud:2020.0033/v1**
  Hamiltonian-Reservoir Replica Exchange and Machine Learning Potentials for Computational Organic Chemistry, R. Fabregat, A. Fabrizio, B. Meyer, D. Hollas, and C. Corminboeuf

  Related MARVEL publication

  R. Fabregat, A. Fabrizio, B. Meyer, D. Hollas, and C. Corminboeuf
  Hamiltonian-Reservoir Replica Exchange and Machine Learning Potentials for Computational Organic Chemistry

  Journal of Chemical Theory and Computation **16**, 3084 (2020).

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

- **10.24435/materialscloud:2020.0031/v1**
  Learning the energy curvature versus particle number in approximate density functionals, A. Fabrizio, B. Meyer, and C. Corminboeuf

  Related MARVEL publication

  A. Fabrizio, B. Meyer, and C. Corminboeuf
  Machine learning models of the energy curvature vs particle number for optimal tuning of long-range corrected functionals

  The Journal of Chemical Physics **152**, 154103 (2020).

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

- **10.24435/materialscloud:2020.0018/v1**
  Surface reconstructions and premelting of the (100) CaF_2 surface, S. Faraji, S. A. Ghasemi, B. Parsaeifard, and S. Goedecker

  Related MARVEL publication

  S. Faraji, S. A. Ghasemi, B. Parsaeifard, and S. Goedecker
  Surface reconstructions and premelting of the (100) CaF_2 surface

  Physical Chemistry Chemical Physics **21**, 16270 (2019).

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

- **10.24435/materialscloud:2020.0014/v1**
  Solvent-mediated morphology selection of the active pharmaceutical ingredient isoniazid: Experimental and simulation studies, D. Han, T. Karmakar, Z. Bjelobrk, J. Gong, and M. Parrinello

  Related MARVEL publication

  D. Han, T. Karmakar, Z. Bjelobrk, J. Gong, and M. Parrinello
  Solvent-mediated morphology selection of the active pharmaceutical ingredient isoniazid: Experimental and simulation studies

  Chemical Engineering Science **204**, 320 (2019).

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

- **10.24435/materialscloud:2020.0013/v1**
  Molecular Dynamics Simulations of Crystal Nucleation from Solution at Constant Chemical Potential, T. Karmakar, P. M. Piaggi, and M. Parrinello

Related MARVEL publication

T. Karmakar, P. M. Piaggi, and M. Parrinello

Molecular Dynamics Simulations of Crystal Nucleation from Solution at Constant Chemical Potential

Journal of Chemical Theory and Computation **15**, 6923 (2019).

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

10.24435/materialscloud:2020.0012/v1

Balancing DFT Interaction Energies in Charged Dimers Precursors to Organic Semiconductors, A. Fabrizio, R. Petraglia, and C. Corminboeuf

Related MARVEL publication

A. Fabrizio, R. Petraglia, and C. Corminboeuf

Balancing Density Functional Theory Interaction Energies in Charged Dimers Precursors to Organic Semiconductors

Journal of Chemical Theory and Computation **16**, 3530 (2020).

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

10.24435/materialscloud:2020.0009/v1

Divalent Path to Enhance p-Type Conductivity in a SnO Transparent Semiconductor, M. Grauzinyte, D. Tomerini, S. Goedecker, and J. A. Flores-Livas

Related MARVEL publication

M. Graužinytė, D. Tomerini, S. Goedecker, and J. A. Flores-Livas

A Divalent Path to Enhance p-Type Conductivity in a SnO Transparent Semiconductor

The Journal of Physical Chemistry C **123**, 14909 (2019).

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

10.24435/materialscloud:2020.0008/v1

Rare-earth magnetic nitride perovskites, J. A. Flores-Livas, R. Sarmiento-Pérez, S. Botti, S. Goedecker, and M. A. L. Marques

Related MARVEL publication

J. A. Flores-Livas, R. Sarmiento-Pérez, S. Botti, S. Goedecker, and M. A. L. Marques

Rare-earth magnetic nitride perovskites

JPhys Materials **2**, 025003 (2019).

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

10.24435/materialscloud:2020.0005/v1

Temperature Dependence of Homogeneous Nucleation in Ice, H. Niu, Y. I. Yang, and M. Parrinello

Related MARVEL publication

H. Niu, Y. I. Yang, and M. Parrinello

Temperature Dependence of Homogeneous Nucleation in Ice

Physical Review Letters **122**, 245501 (2019).

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

github.com/BarakHirshberg/PIMD_for_fermions_data

PIMD_for_fermions_data, B. Hirshberg

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Open-shell Non-benzenoid Nanographenes Containing Two Pairs of Pentagonal and Heptagonal Rings, J. Liu, S. Mishra, C. A. Pignedoli, D. Passerone, J. I. Urgel, A. Fabrizio, T. G. Lohr, J. Ma, H. Komber, M. Baumgarten, C. Corminboeuf, R. Berger, P. Ruffieux, K. Müllen, R. Fasel, and X. Feng

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Geometric landscapes for material discovery within energy-structure-function maps

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

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Large magnetoresistance and nonzero Berry phase in the nodal-line semimetal MoO_2, Q. Chen, Z. Hou, S. Zhang, B. Xu, Y. Zhou, H. Chen, S. Chen, J. Du, H. Wang, J. Yang, Q. Wu, O. V. Yazyev, and M. Fang

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Project Inc1

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L. Talirz, S. Kumbhar, E. Passaro, A. V. Yakutovich, V. Granata, F. Gargiulo, M. Borelli, M. Uhrin, S. P. Huber, S. Zoupanos, C. S. Adorf, C. W. Andersen, O. Schütt, C. A. Pignedoli, D. Passerone, J. VandeVondele, T. C. Schulthess, B. Smit, G. Pizzi, and N. Marzari
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Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds, N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi, and N. Marzari

Related MARVEL publication

L. Talirz, S. Kumbhar, E. Passaro, A. V. Yakutovich, V. Granata, F. Gargiulo, M. Borelli, M. Uhrin, S. P. Huber, S. Zoupanos, C. S. Adorf, C. W. Andersen, O. Schütt, C. A. Pignedoli, D. Passerone, J. VandeVondele, T. C. Schulthess, B. Smit, G. Pizzi, and N. Marzari
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Group(s): Marzari, Passerone, Pizzi, Schulthess, Smit, VandeVondele / Project(s): DD4, OSP, HPC

Annex 3 Status of structural measures implementation

Planned measures according to annex 3 of the NCCR contract for phase 2	Current status of implementation and comments
Infrastructure	
Additional measures	
250'000 CHF in cash for data storage and services for Materials Cloud	Ongoing
Faculty	
Planned new professorship	
New Assistant professor (PATT) in Computational Materials Science (Institute of Materials), planned for 2020	The call was open, deadline for submission of applications December 14, 2020, interviews scheduled between February 22 and March 5, 2021
Continuation of professorships of phase 1	
- Michele Ceriotti	Ongoing, appointed as Associate Professor (September 2020)
- Oleg Yazyev	Ongoing, appointed as Associate Professor (September 2020)
- Martin Jaggi	Ongoing

Specific conditions and requirements according to Article 10 of the NCCR contract for phase 2	Current status of implementation and comments
Equal opportunities, analysis and plans	The implementation of the new initiatives has started. The details are given in Section 5.3 Equal opportunities

Cover picture

AiiDA provenance graph (100'000+ nodes) representing the workflows deployed to assess carbon-capture performance in 324 covalent-organic frameworks (Berend Smit group and Open Science Platform).

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