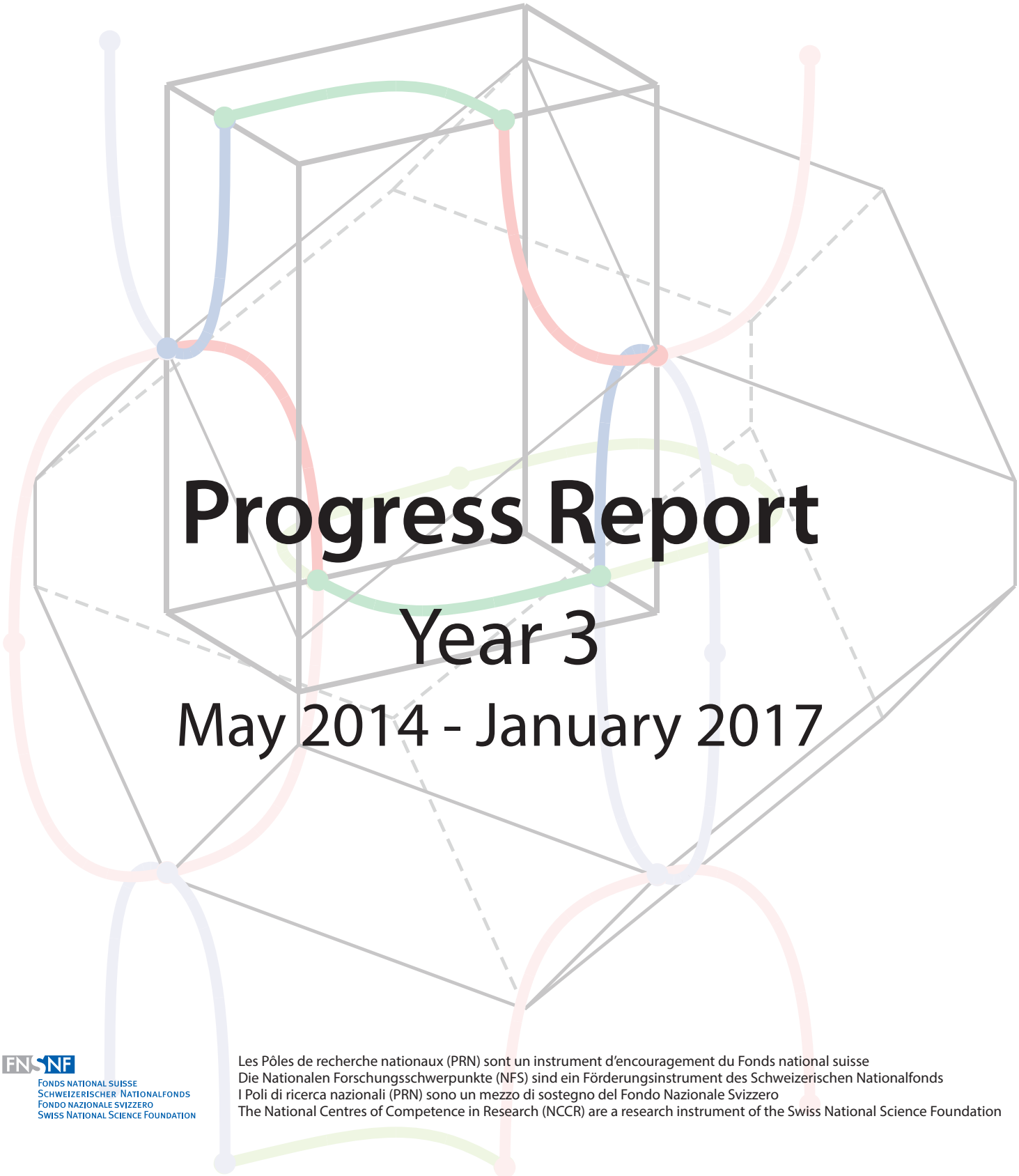
MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Materials' Revolution: Computational Design and Discovery of Novel Materials



Progress Report

Year 3

May 2014 - January 2017

FNSNF
Fonds national suisse
Schweizerischer Nationalfonds
Fondo nazionale svizzero
Swiss National Science Foundation

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Programmes division
National Centres of Competence in Research

NCCR: 3rd Progress Report - Cover Sheet

Title of the NCCR	Materials' Revolution: Computational Design and Discovery of Novel Materials (MARVEL)
NCCR Director Name, first name Institution	 Marzari, Nicola EPFL, Lausanne
Date of submission	February 19, 2017

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This report follows the new guidelines for size limits introduced this year by the SNSF.

1 Executive summary

MARVEL started in 2014 with a mission of computational design and discovery of novel materials. In the first phase, it has been growing, maturing, and creating a community, with groups searching and developing new synergies and learning how to tackle the challenges of materials design and discovery. It has also been developing the computational tools, the informatics framework, and the experimental collaborations to engage in the ambitious grand-challenge projects of phase 2. The management areas supported by MARVEL have been especially beneficial for these goals — from the all-hands meetings and retreats to the junior retreat to EPFL's junior seminars and distinguished lectures. Outstanding scientific results have been obtained, e.g. for topological materials with novel electronic structure and transport properties [4-7, 9, 10, 21], for metal-organic perovskites tailored for photovoltaic efficiency and enhanced stability [30-34], or for one- and two-dimensional materials, with exquisite control on synthesis and with novel candidates for electronic, optical, and magnetic properties [60, 62, 63, 70, 73]. A core strength of the project lies also in the careful development of complex techniques for modeling, as can be seen in outputs that are at the intersection of vertical and horizontal projects — from d-wave superconductivity to homogeneous catalysis to aqueous redox systems (e.g. [19, 38, 54, 89, 111]) — or that push electronic-structure techniques — from weak and strong correlations to enhanced scalability of wavefunction methods (e.g. [79, 83, 84, 86]). The new field of materials' informatics is showing more and more its relevance for the project (e.g. [123, 124, 136, 138]), as are the contributions in developing the optimal hardware and software platforms for high-performance and high-throughput computing, or for the verification and validation of calculations [59, 121, 143-145]. In this report we also see the first results from the joint experimental and computational projects of PP7: all 14 have started, and the enthusiasm of the experimental counterparts is shown by the commitments for phase 2, laying the cornerstone for the future projects. Last, a complete management team and full set of PIs for the 4 management areas is now allowing coherent development and strategic efforts in all of these.

Vertical Project 1: Novel Materials Physics The key research question in VP1 has been how to achieve new phases of matter with desired magnetic, electronic or topological properties in a predictable manner using chemistry, structure, heterostructuring or strain-control as design parameters. In transition-metal oxides we have solved long-standing problems of how to describe the electronic structure of the correlated systems such as rare earth nickelates and d^1 and d^2 titanates and vanadates. We have identified an entirely new mechanism for forming polar magnetic spirals in disordered oxide materials which has led to the joint theoretical-experimental realization of a room-temperature multiferroic material. And we have created new designer materials with specific model Hamiltonians to study exotic fundamental physical behaviors. The discovery of novel topological materials has been enabled by the development of algorithms and computer codes for identifying topological features in band structure, and notably by the integration of Z2PACK and WANNIER90. New topological electronic phases, namely the type-II Weyl semimetals, triple point and nodal chain metals, have been found. First-principles high-throughput screening of databases of known compounds has revealed a number of new candidate topological materials, some of which have already been realized experimentally.

Vertical Project 2: Novel Materials Applications The VP2 project is focusing on four grand-challenge problems, which consist in identifying optimal materials for solar cells, for water-splitting catalysts, for solid-state ionic conductors, and for low-dimensional materials. Each of the research teams involves researchers from VP2, from the horizontal projects of MARVEL, and experimental partners. All projects are growing towards material searches on databases through the AiiDA platform (PP6). The scientific output achieved so far is impressive. However, the full poten-

tial of VP2 still lies ahead, as the synergies continue to grow and the material searches enter an operative phase.

Horizontal Project 3: Advanced Quantum Simulations We developed efficient continuous-time quantum Monte Carlo methods for correlated lattice fermions and designed an approach to compute fidelity susceptibility for correlated materials. A consistent GW+DMFT scheme, which treats different orbitals with an appropriate level of accuracy, was developed and implemented. We enabled simulations of electrochemical processes using MP2 and RPA and simulated aqueous redox systems by molecular dynamics and Monte Carlo using these methods.

Horizontal Project 4: Advanced Sampling Methods New and improved methods were developed to sample the potential energy landscape. First applications were done to help solving some of the key MARVEL challenges such as better materials for photovoltaics or for carbon capture. A common theme for all these efforts are quantities that allow to characterize materials. Depending on the context these quantities are called fingerprints, descriptors or collective variables. Work has started to compare the various fingerprints used by different groups and to assess whether they can also be used in other contexts. Methods that allow to study nucleation and growth will give guidance to synthesis efforts.

Horizontal Project 5: Materials Informatics The goal of HP5 is to develop data driven methodologies for the acceleration of material discovery. The scientific community has been generating enormous amounts of valuable knowledge that has mostly remained confined into papers. Recently, it became evident that the data driven approach can unlock the huge potential of this data and allow for drastic acceleration of discovery. Indeed, HP5 researchers demonstrated that machine learning models can provide very accurate predictions of materials properties at a fraction of the cost and time needed by traditional approaches. Extracting the scientific literature treasure and structuring into searchable forms allow researchers to very fast learn from the collective experience of the community and thus move forward much faster. This is of course only the beginning. We have merely scratched the surface and already gotten strong evidence of the full potential of the approach.

Platform Project 6: Informatics The Informatics platform is delivering, ahead of schedule, its objectives of 1) developing a materials' informatics infrastructure to manage high-throughput calculations, organize all data with full provenance and reproducibility, and encode in robust workflows the calculation of complex materials properties that also allow for continuous testing and verification and validation of the calculations; 2) developing a portal for the dissemination and sharing of the curated data, of the entire provenance and data tree, and also of educational materials and work tools for the community (additional objective with respect to the original proposal); 3) developing a shared software infrastructure, in the form of the SIRIUS domain-specific library, able to unlock the power of emerging supercomputing platforms based on multi-core, GPU, and accelerator architectures; and 4) verifying and validating the calculations, by comparing with all-electron and experimental results. These objectives are also supported by a close participation of CSCS staff in provisioning of services and shared solutions.

Platform Project 7: Experiments All 14 new collaborations between computational and experimental partners have started, covering a broad range of topics related to VP1 and VP2. Among the first exciting results are the confirmation of a novel topological material, new insight into the relationship between thermodynamics, chemical stability and water splitting activity of Ru-based perovskites, and the input for refinements of Co_4O_4 catalytic cycles.

Management areas For KTT, the AiiDA platform is reaching maturity, and is being adopted by many groups inside and outside MARVEL; the Materials Cloud portal is now the focus of our effort, preliminary to the Open Science platform of phase 2. Close synergy with CSCS is in place, not only to optimize hardware performance, but to develop the software solutions needed for high-throughput computing, long-term storage, and authorization. The industrial outreach has been steadily increasing, thanks to a deeper and coherent portfolio of research projects and directions. In education, the junior retreat and the MARVEL contributions to the extended 2-week colleges and schools in Trieste, Accra, and Khartoum have been particularly successful and satisfactory. In equal opportunities, the well established efforts for the younger generations are now complemented by the INSPIRE Fellowships and will also see a high-school camp in 2018. In communication, the junior seminars and the distinguished lectures are all established and very successful.

2 Reaction to the recommendations of the review panel

We took each and every recommendation of the review panel at heart, and here we present our actions in response to those, starting from the final recommendations of the 2^{nd} year report.

The NCCR should take on collaborative grand challenges. Collaborative projects should be rewarded and especially young people should be promoted and encouraged with increased funding if at all possible.

The first phase of MARVEL has been dedicated to aligning the computational community within this project to the theme and the challenges of materials discovery while also creating a common informatics platform. We think that this phase was prerequisite for the next step, where more ambitious design-and-discovery projects take place. To accelerate this transition, we have embraced this request and have changed the structure of the project:

- First, the pre-proposal of phase 2 has been designed explicitly around collaborative grand challenges — major "design and discovery projects" that involve multiple computational and experimental groups. Each of these focuses on a particular topic that is of significant interest for potential applications.
- Second, we have stressed the core goals of collaborations in phase 1, and as an outcome of the year 2 review, projects have worked to sharpen their focus and to create new synergies, especially in VP2 and in HP4, discussed later. In addition, we will present all the joint efforts with posters during the site visit, to allow for a fine-grained display of the ongoing collaborative work.
- Third, we have reallocated 1 M CHF of the budgeted funding, to promote and encourage young or new investigators. Thanks to this effort, we were able to launch 6 "Agility Plus" projects in Jan 2017 (as detailed in Chap. 4.2, led by new or young PIs: Aschauer, Ceriotti, Passerone, Smit, von Lilienfeld, and Yazyev), that will be followed by 2 more in May 2017; a prerequisite for those was to be collaborative and to work on dissemination through the Materials Cloud portal, so that these groups can build synergies and develop the expertise for the Open Science platform of phase 2.
- Last, we have included in MARVEL a new tenure-track professor in machine learning (Martin Jaggi, EPFL), a new SNSF professor in functional oxides (Ulrich Aschauer, UniBE), and a new senior PI with extensive track-record in collaborating with the industry (William Curtin, EPFL), also to compensate for the new leadership positions taken elsewhere by Matthias Troyer (Microsoft), Antoine Georges (Simons Foundation) and Joost VandeVondele (CSCS), for the retirement of Wanda Andreoni, and the leave of Christoph Koch (discussed in more detail in Chap. 3).

Feedback from engineering, industry and experiments should be encouraged. Experiments should be empowered to challenge theory.

- Close experimental collaborations are a prerequisite for the grand-challenge projects of phase 2, with an additional significant effort in injecting the challenges from engineering and industry in the Bonus Project, dedicated to additive manufacturing. The enthusiasm and support of the experimental community is continuing thanks to the very successful groundwork of PP7, addressing now larger and more articulated efforts. This enthusiasm can also be seen by the pledge of the Paul Scherrer Institute to match MARVEL funding by allocating an additional 2 M CHF in cash for MARVEL for joint activities in phase 2.

The structure-related activities (KTT, education and training, equal opportunities, communication) need to extend the participation of groups other than that of EPFL.

- We now have a coherent leadership in the 4 management areas, that also benefits from the increased workforce coming from the successful hire of Dr. Nathalie Jongen as program manager (50% FTE), bringing with her the experience of the CCMX Centre for Materials Science and Technology (2006 – 2016). KTT, in addition to Marzari and van Landuyt (EPFL), has now Passerone, at Empa, whose focus on knowledge transfer is enhanced by the collaboration with the Empa-Akademie (e.g. Passerone organized in Feb 2017 a workshop on "Modeling and Simulation in Industrial Research"). In education, Smit and Jongen are complementing Ceriotti, and are actively working with EPFL to create a dedicated semester to advanced modeling classes at all scales. In equal opportunities Hutter (UZH) has joined the EPFL team of Corminboeuf, Favre-Quattropani and Füger. The INSPIRE Fellowships program has an evaluation committee composed of Ceriotti, Spaldin (ETHZ), Werner (UniFR) in addition to the EPFL team. In communication, Pasquarello, Jongen and Favre-Quattropani are now complemented by Yazyev and De Lorenzi (deputy director of CSCS). Last, a major effort of all the computational PIs in MARVEL covers KTT through the development, dissemination, and training in open-source software and advanced simulations techniques — we present a list of the activities organized or sponsored on nccr-marvel.ch/ctw.

When shaping the program for the next phase, the potential and willingness of the PIs for entering new collaborations and tacking novel questions should be an important criterion.

- We have set up a competitive process for phase 2, where the 7 grand-challenge design and discovery projects will compete for 5 slots. The feedback of the review panel will be taken into consideration, and a final decision will be made, together with the Scientific Advisory Board, at the Review and Retreat of Sep 2017. We believe that injecting such competitive mechanism into the selection process will allow to see clearly which are the most ambitious and collaborative projects that are responding to the metrics of MARVEL.

The budget for the second phase of the NCCR should foresee more financial flexibility to increase the dynamics and the ability of the Director and the Executive Committee to steer and guide the NCCR.

- The major design and discovery projects that will be approved for start in the second phase will have a budget of 2 years and will need to have experimental results within this timeframe; continuation will only be granted upon successful review by the SNSF Panel and the Scientific Advisory Board. The incubator projects in phase 2 will have a lifetime of 2 years.

Also, we will comply with the requests for the site visit — from joint posters to presentations organized around cross-cutting topics to time-keeping and PIs attendance.

Last, we provide here a detailed response to the different comments of the Panel to the individual projects and to the different management areas.

VP1

A number of measures has already been taken in order to address the recommendations of the review panel. Oleg Yazyev, the junior participant of VP1, received supplementary funding via an "Agility Plus" grant for implementing the computational workflow (AiiDA) and data infrastructure (Materials Cloud) for the high-throughput search of topological materials. The members of VP1 are actively developing further collaborations within the NCCR (e.g. Yazyev with the group of Marzari) and receiving feedback from experimental partners (e.g. the group of Ming Shi) with regard to establishing the target properties of topological materials. The comments on ammonia and water catalysts are addressed in VP2, below.

VP2

General/VP2: Grand-challenge problems and collaborations. After an initial phase in which each group has built up its individual expertise, VP2 has now reached a stage in which well defined projects emerge, in which grand-challenge problems can be addressed through a collaborative effort. The structure of VP2 has been reorganized accordingly. Additionally, this reorganization will form the basis for con-

tinuation of the projects in MARVEL phase 2. The four grand challenges are:

1. *Perovskites for photovoltaic applications*, led by Röthlisberger, with von Lilienfeld, Goedecker, Ceriotti, Parrinello, and Pasquarello. Grand challenge: Understanding growth to design a highly efficient and stable perovskite for light harvesting purposes. Experimental partners: Grätzel (EPFL)

2. *Superior electrocatalysts for oxygen evolution and other fuel cell reactions*, led by Corminboeuf, with Pasquarello, Marzari, Hutter,von Lilienfeld. Grand challenge: Design of next-generation catalysts. Experimental partners: Hu (EPFL), Schmidt and Fabbri (PSI).

3. *Low-dimensional materials*, led by Passerone, with Marzari, Tavernelli, Hutter. Grand challenge: Low-dimensional materials from high-throughput screening to working devices. Experimental partners: Fasel (Empa).

4. *Ion conductors*, led by Laino, with Marzari, Smit, Ceriotti. Grand challenge: Search for optimal ion conductors. Experimental partners: Lippert and Pergolesi (PSI).

General: Engineering and technology challenges. Every grand challenge works in close interaction with an experimental team, which guides the project from the very beginning towards achievable technological applications.

VP2: Absence of synergy in the project on "CO_2 capture in ammonia". This project was supporting W. Andreoni and following her retirement will be discontinued starting December 2016.

VP2: Absence of synergy in the project "Surface deterioration studies of water catalysts". This project will be incorporated in the grand challenge "Superior electrocatalysts for oxygen evolution reaction" and will thus naturally benefit from the collaborative framework that has been set up for addressing this particular grand challenge.

VP2: Projects are scattered. The new organization around four selected grand challenges responds to this criticism.

VP2: Synergistic collaborations are recommended. The number of synergistic collaborations has grown considerably in year 3. Furthermore, the new structure of VP2 around a set of well-chosen grand-challenge problems emphasizes the collaborative efforts.

VP2: Postdocs do not know what is going on in MARVEL. A variety of channels for interactions between postdocs and PhD students have been set up with the MARVEL project. At the annual junior retreat, they meet in a self-organized fashion to share the progress achieved among the various MARVEL groups. Furthermore, topical groups of postdocs and PhD students get to know each other in various MARVEL supported events, such as AiiDA schools, AiiDA programming sessions, and international conferences (e.g. Workshop in Ascona, *Nothing is perfect – the quantum-mechanics of defects*). The enhanced collaborative research activity amongst PIs in year 3 further allows these young researchers to naturally interact and share their results. In addition, starting Nov 2016, postdocs and PhD students at EPFL meet on a regular basis at the junior seminars to expose and debate their results, sometimes joined by young researchers from outside EPFL. All these channels of interaction will contribute to creating a vibrant MARVEL community. The new structure emphasizing collaborations in MARVEL phase 2 will further contribute to the establishment of links among the junior researchers.

VP2: The work on water splitting appears as being incoherent. In this initial phase, the research activity on water splitting has been to some extent explorative and has developed along two directions. The first direction concerns "electrocatalysis" on both solid-state (Corminboeuf, Pasquarello) and molecular catalysts (Corminboeuf, Hutter) for water oxidation and reduction. The second direction concerns the examination of various "electronic structure methods" (Marzari, Pasquarello) for the accurate description of energy-level alignment. These activities are coming together in year 3 of MARVEL and are instrumental to address the grand challenge on "Superior electrocatalysts for oxygen evolution reaction".

HP3

More communication between the two distinct efforts on strong correlation lattice models and weakly correlated ab initio-modeled systems would be desirable. The review panel is correct that communication between groups working on strong and weakly correlated methods has not been improved substantially. It was foreseen in the original proposal that such collaborations would emerge but up to now only marginal exchange happened. The reasons for this are probably manyfold. On the one hand, we experience boundaries due to language problems (physics vs chemistry, strong vs weak correlation). On the other hand, there are also differences in focus, e.g. qualitative understanding through models vs large-scale simulations using refined codes for high-performance computing. Still, we have made several attempts to bridge the problems and work out common projects. It may be that inclusion of intermediates from the field of static correlation from quantum chemistry (e.g. the Reiher group using DMRG) might help. Such contacts exist from both ends (see also [1]). The most promising route will be to identify a clearly defined problem that would be out of reach for any individual effort, thus needing a collaboration.

HP3 is really crucial to this center and should be more dynamic and possible these two efforts should interact more. We believe that except for the missing deeper interaction already discussed above, the individual teams of two PIs and their groups showed with their common results that strong interactions exist and have positive effects. Of course, it is always desirable to be more dynamic in any research environment. However, it has to be kept in mind, that method development is tedious and requires a lot of effort to develop, implement, and test new algorithms to the point that they are not just proof of concepts, but can be safely used also by users.

It is recommended that junior people get more opportunity to drive and innovate. It is not clear if the review panel is here referring to junior members of the research groups or the involvement of junior PIs. For the first case, we believe that PhD students and postdocs are certainly getting the guidance and help needed to prosper in this competitive and challenging field. The PIs also give them the freedom to bring up new ideas and in fact support any initiative in this direction. The situation regarding junior PIs is unfortunately not so positive (see also below). Since the start of the SNF assistant professor program 15 years ago, there was no single award to a computational chemist in electronic structure development. Previous awardees in physics are now senior PIs in MARVEL (Troyer and Werner). Some of the junior PIs working within MARVEL do have interests in electronic structure development, but mostly concentrate on topics related to other projects within VP1 (Yazyev), VP2 (Corminboeuf), and HP5 (Ceriotti, von Lilienfeld). We hope that through the already started and possible future collaborations with them, also HP3 can benefit from their new ideas and enthusiasm.

. . . Information from experiments — When does theory fail? What is needed to make accurate predictions? — to drive innovation in theory is desirable. Interaction with experiments is crucial for all forms of simulation and theory. The PIs of HP3 are aware of the importance of new experimental findings and see their work driven by documented failures of theory/simulations and the need to support experiment with more accurate predictions. However, the current setup of the experimental platform PP7 within MARVEL aims at different goals. The projects were chosen to optimally advance the materials discovery goal of MARVEL and not to contribute to or test specific theoretical questions.

Concern was also expressed that Joost VandeVondele may move due to inherent uncertainty of his position. Unfortunately, we were not able to keep Joost VandeVondele in HP3 and he has recently left ETHZ for CSCS. This is a great loss for the project and it will be difficult to find an adequate replacement.

HP4

We have put forward a strategy to further strengthen the collaborations in HP4. In one such effort, we will focus on a common topic of all HP4 groups, namely fingerprints. We started already sharing both our datasets and different fingerprint technologies. The analysis of our findings is ongoing and a common publication comparing the various fingerprints is planned. Various activities are also ongoing, or will be started soon, to support the research on perovskites in VP2. In collaboration with the Röthlisberger group, the Parrinello group started simulations to understand the nucleation and growth of perovskites. The Goedecker group will perform further structure predictions of more complex perovskites (such as mixed organic inorganic perovskites). The von Lilienfeld group will develop machine learning schemes for these perovskite materials.

HP5

The members of HP5 thoroughly discussed the recommendations of the review panel. It was clearly understood that the reviewers strongly encouraged deeper collaborations, both within HP5, as well as across MARVEL. In addition, the review panel would like to see a clear link of the cognitive work with the rest of the project. We have taken a very active approach in order to implement these recommendations. We started a number of key collaborations with VP2 (Marzari) for the integration of the AiiDA platform and (Spaldin) to expand the knowledge graph to other fields of interests, such as multiferroic systems with the help of CSCS (Schulthess) and ETHZ library. In these collaborations, the cognitive engine that extracts needed knowledge from scientific literature and organizes it into a searchable structure (e.g. a knowledge graph) is central. We plan a major demo for the review panel in Apr 2017. In addition, we organized regular discussions and site visits of HP5 members to other groups as well as participation to all MARVEL related events (schools/retreats).

PP6

The review panel was overall very positive about this project; we would like to underline that the platform is reaching maturity. Many groups within MARVEL, MaX, and the broader community have been developing plugins, workflows, and using it for high-throughput searches.

PP7

For the evaluation of the future of PP7 within MARVEL phase 2, the recommendation for addressing real challenges has been taken into account. At the current stage, with all PP7 subprojects running, we will continue to jointly work together and have a feedback from the experiments which might challenge the theory or vice versa.

Knowledge and technology transfer

We thank the panel for the positive feedback, and we will focus more and more our efforts towards industrial outreach. Having Dr. Van Landuyt dedicate 1 day/week to MARVEL activities has been a great help, and it is significantly increasing our visibility and our strategy and portfolio in engaging industrial partners.

Education and training

We appreciate the positive feedback re the junior retreat, and, in response to the comments, for the junior retreat of summer 2016, the organizers set up 8 teams of 6 people each, with the challenge of brainstorming and proposing a possible research project for MARVEL — topics went from "intelligent solar panels" to "scalable quantum computing". 6 of the teams presented during the Review and Retreat their elevator pitches, followed by Q&A, for possible phase 2 research projects; ideas from two groups were incorporated in the pre-proposal of phase 2. This effort will continue both at the junior retreat and in the different MARVEL meetings.

Equal opportunities

We thank the panel for the positive feedback regarding all the activities, that will continue while also expanding our effort in the INSPIRE Fellowships for women, an inter-NCCR initiative in collaboration with the NCCR QSIT. In response to the comment on broadening sensitivity to equal opportunities, it is the vision of the Director that EPFL should start offering a 3-hour training to all incoming personnel focused on gender and ethics — in parallel to the 3-hour training on safety that every new arrival at EPFL is obliged to take (*formation obligatoire de base en sécurité*). The equal opportunity team is working on a pilot project on this, involving MARVEL personnel.

Communications

We thank the panel for the positive feedback; the arrival of Dr. Jongen as program manager is also helping us a lot, with a newsletter, monthly highlights, and improved web content in the works. In addition, the Materials Cloud portal will also help making our effort visible and distributing software and educational material.

3 Management

3.1 Structure and organisation of the NCCR

3.1.1 Structure of the NCCR

NCCR MARVEL is organized around 2 vertical projects of materials design and discovery, focusing on novel materials physics (VP1) and novel materials applications (VP2), supported by 3 horizontal projects on advanced quantum simulations (HP3), advanced sampling methods (HP4), and materials informatics (HP5), that are interfaced to 2 platform projects on the informatics infrastructure (hardware and software) (PP6) and on the experimental pipeline (PP7). EPFL is the home institution and participating scientists are affiliated with 12 Swiss academic and industrial institutions — with the University of Bern joining in Jan 2017 — forming a strong network in the field of computational design and discovery of novel materials. MARVEL is organized around three bodies responsible of its operation, the Executive Committee, the Scientific Committee and the Scientific Advisory Board. This year, the Executive Committee was reinforced with a fourth member — Berend Smit (EPFL); the other members are Nicola Marzari (EPFL), Alfredo Pasquarello (EPFL) and Thomas Schulthess (ETHZ and CSCS); the Scientific Committee is unchanged from the previous report; the members of the Scientific Advisory Board and members of the scientific projects can be found in the website.

3.1.2 Organisation of the NCCR

As planned, 7 more experimental group leaders — Raffaella Buonsanti (EPFL), Daniele Pergolesi (PSI), Wendy Queen (EPFL), Marco Ranocchiari (PSI), Marta D. Rossell (Empa), Christian Rüegg (PSI) and Ming Shi (PSI) — entered the experimental platform PP7 with new 2-year projects. Joost VandeVondele left ETHZ in Oct 2016 and he is now heading the Future Systems group at CSCS; he will still be closely involved in MARVEL through the participation of Thomas Schulthess. Christoph Koch is on a 1-year sabbatical leave, and it was mutually decided to stop funding in years 3 and 4. Matthias Troyer is on a 2-year leave in the Quantum Architectures and Computation Group, of Microsoft Research, part of a major effort of Microsoft to develop quantum computing; the activity on topological insulators will continue strongly at ETHZ, and for the rest of phase 1 Olef Yazyev will replace him as co-project leader in VP1, together with Nicola Spaldin. Also, Antoine Georges will direct, from Sep 2017, the new Center for Computational Quantum Physics in New York City, funded by the Simons Foundation. These last two are actually examples of how strong the MARVEL community is, and will lead to additional important international synergies. Three new members will enter MARVEL through the collaborative "Agility Plus" effort discussed in Chap. 2 and 4.2: Ulrich Aschauer (UniBE) in Jan 2017, and William Curtin (EPFL) and Martin Jaggi (EPFL) in May 2017 (the six new "Agility Plus" projects started in Jan 2017 are led by Aschauer, Ceriotti, Passerone, Smit, von Lilienfeld, and Yazyev; two more will start in May 2017, led by Curtin and Jaggi).

There are several changes to the management team: Ursula Vaucher, responsible for financial reporting of MARVEL and who is affiliated with the EPFL Research Office, replaced Valérie Le Dreau in Feb 2016. Nathalie Jongen joined MARVEL in Jun 2016 as program manager, bringing her extensive experience in managing the CCMX Competence Centre for Materials Science and Technology. Elizabeth Gueniat, administrative assistant, retired at the end of May 2016; she was replaced by Nicoletta Isaac from Aug until Dec 2016; Monika Salas-Tesar serves in the interim and Claire-Lyse Rouiller will start in April 2017. The

4 management areas have, as detailed in the previous chapter, Marzari, Passerone, and van Landuyt in KTT, Smit, Ceriotti and Jongen in education and training, Corminboeuf, Hutter, Favre-Quattropani and Füger in equal opportunities, and Pasquarello, Yazyev, De Lorenzi, Favre-Quattropani, and Jongen in communication.

3.2 Management activities and status of collaboration/integration

3.2.1 Activities and measures

Events organisation

In this third year, the management organized meetings, lectures and events that are described in chapters 5 to 8; we e.g. mention:

- Ig Nobel Award Tour Show on the EPFL campus, Mar 23, 2016.
- Review Panel meeting at EPFL, Apr 19 – 20, 2016.
- Inauguration of the ME D building at EPFL, May 10, 2016.
- Platform for Advanced Scientific Computing PASC16 Conference organized by CSCS at EPFL, Jun 8 – 10, 2016, with a booth and a poster presenting MARVEL.
- INSPIRE Potentials — MARVEL Master Fellowships for female Master students.
- MARVEL/MaX/Psi-k tutorial on high-throughput computations: general methods and applications using AiiDA at EPFL, Jun 22 – 24, 2016.
- Second MARVEL junior retreat in Les Diablerets, Jul 18 – 21, 2016, with 48 participants.
- Third MARVEL Review and Retreat, gathering annually all MARVEL members, Sep 7 – 8, 2016 at EPFL, with 112 participants, including 4 Scientific Advisory Board members.
- Photography exhibition by Julie Birenbaum at EPFL, from Sep 8, 2016.
- ECAM "WANNIER90 Software Development Workshop" conference in San Sebastian (SP), Sep 12 – 19, 2016, logistical and financial support.
- MARVEL booth at EPFL Open Days, Nov 5 – 6, 2016.
- AiiDA coding week in Leysin, Dec 5 – 9, 2016.
- 2 MARVEL distinguished lectures at EPFL: Prof. Clare P. Grey (Univ. Cambridge, UK), Oct 26, 2016, and Prof. Laura Gagliardi (Univ. Minnesota, USA), Dec 20, 2016. A lecture by Prof. Annabella Selloni (Princeton Univ.) is already planned for May 16, 2017.
- 3 MARVEL junior seminars at EPFL, Nov 17, Dec 15, 2016, and Jan 19, 2017, continuing on a regular monthly basis.
- 3 meetings with the computational group leaders and the 3 PP7 leaders in Bern, Jul 21, Nov 4 and Dec 14, 2016.
- 14 seminars at EPFL.

Other activities

MARVEL members organized 17 conferences, tutorials or workshops (not counting the AiiDA tutorials), of which MARVEL sponsored 11. The Psi-k Network and the QUANTUM-ESPRESSO Foundation were supported through group membership fees.

Measures

The management team is working on a *welcome letter* addressed to all new MARVEL members that will include information and requirements regarding finances, acknowledging MARVEL in publications, visual identity (e.g. usage of logos), gender issues, tech transfer, etc.

3.2.2 Status of collaboration/ integration

The management team is finally fully in place, with very experienced personnel, and that will be of great help in running the project; same can be said for the people in charge of the management areas. The arrival of Smit in the executive committee has also been very welcome and stimulating. Most importantly, the meetings, retreats, and reviews are building a sense of community and true collaborations with different groups that are exclusively the result of MARVEL — these will be highlighted especially in the poster session of the April site visit, but we are seeing this very clearly at many levels — from group leaders to students and postdocs, and also between different institutions, with e.g. PSI, Empa and CSCS having developed many new links with groups at EPFL, ETHZ, and all the other Universities involved.

4 Research

4.1 Results over the past 33 months

Vertical Project 1 — VP1 — Novel Materials Physics

Project leaders: Matthias Troyer (ETHZ), Nicola Spaldin (ETHZ)

Participating members: Matthias Troyer (ETHZ), Nicola Spaldin (ETHZ), Antoine Georges (UniGE), Oleg Yazyev (EPFL)

Summary and highlights: The key research question in VP1 has been how to achieve new phases of matter with desired magnetic, electronic or topological properties in a predictable manner using chemistry, structure, heterostructuring or strain-control as design parameters. In transition-metal oxides we have solved long-standing problems of how to describe the electronic structure of the correlated systems such as rare earth nickelates and d^1 and d^2 titanates and vanadates. We have identified an entirely new mechanism for forming polar magnetic spirals in disordered oxide materials which has led to the joint theoretical-experimental realization of a room-temperature multiferroic material. And we have created new designer materials with specific model Hamiltonians to study exotic fundamental physical behaviors. The discovery of novel topological materials has been enabled by the development of algorithms and computer codes for identifying topological features in band structures. New topological electronic phases, namely the type-II Weyl semimetals, triple point and nodal chain metals, have been found. First-principles high-throughput screening of databases of known compounds has revealed a number of new candidate topological materials, some of which have already been realized experimentally.

1 Main goals and achievements

For the correlated materials part of VP1, the main phase 1 achievements have been the understanding of the low-energy physics of the nickelates as well as d^1 and d^2 t_{2g} perovskites, and the design of a new class of room-temperature multiferroics with an entirely new mechanism for stabilizing spiral magnetic order. In addition, our rational design approach has been illustrated with the prediction of new materials with unusual yet appealing Hamiltonians — in one case the single-band Hubbard model, and in another, strong coupling between structural Higgs and Goldstone modes — which are currently being sought experimentally. As far as the topological materials part of VP1 is concerned, the phase 1 goals can be concisely summarized as searching for novel topological electronic phases, establishing a methodology for identifying these topological electronic phases in materials, development of protocols for the high-throughput search of topological materials, and eventually experimental confirmation of selected candidate materials.

1.1 Materials discovery

Novel materials have been discovered, e.g. the strong topological insulator β-Bi_4I_4 characterized by the low density of intrinsic charge carriers as well as materials realizing novel gapless topological phases. Materials realizing

other topological phases, e.g. Chern insulators, are expected to be confirmed by the end of phase 1. In addition, new materials have been proposed — in particular single-band Hubbard model material — that are awaiting experimental verification.

1.2 Novel phenomena

As well as the design of new materials with specific functionalities, a goal of VP1 is to identify new physical phenomena. Here two examples stand out: our new route to high-temperature spiral magnets, and hence high-temperature multiferroics, driven by disorder-based frustration, and our identification of the hexagonal manganites as a materials system demonstrating coupled Higgs/Goldstone behavior.

1.3 High-throughput search

High-throughput classification of topological materials is advancing as planned. A database containing these results is expected to be made publicly available by the end of phase 1.

2 Scientific outputs

The research in topological materials has resulted in a number of publications in high-impact journals, including *Nature* [2, 3], *Nature Materials* [4], *Nature Communications* [5], *Physical Review Letters* [6, 7, 8] and *Physical Review X* [9, 10]. Matthias Troyer has been awarded the 2016 Aneesur Rahman Prize for Computational Physics of the American Physical Society for his work on numerical simulations of quantum systems. Nicola Spaldin has been awarded The L'Oréal-UNESCO Women in Science Prize (2017), Lise Meitner Lecturer of the German and Austrian Physics Societies (2017), Körber European Science Prize (2015) and ETHZ Golden Owl for teaching excellence (2014). Antoine Georges was elected to the French Academy of Sciences in 2014 and received the Hamburg Prize for Theoretical Physics (2014).

3 Progress of the different efforts

3.1 The rare earth nickelates (Antoine Georges — UniGE, Nicola Spaldin — ETHZ, Marisa Medarde — PSI)

The series of rare earth perovskite nickelates, $R\mathrm{NiO_3}$, exhibit a complex phase diagram where all members except $\mathrm{LaNiO_3}$ undergo a metal-insulator transition (MIT) accompanied by a structural distortion. This "breathing mode" distortion leads to alternating large and small oxygen octahedra surrounding the $\mathrm{Ni^{3+}}$ cations on adjacent sites. At low temperatures, a magnetically ordered antiferromagnetic (AF) phase with wave-vector $\boldsymbol{k} = (\frac{1}{4}\,\frac{1}{4}\,\frac{1}{4})$ (in pseudo-cubic units) occurs. For $\mathrm{NdNiO_3}$ and $\mathrm{PrNiO_3}$ the MIT coincides with the AF transition, whereas for all other members of the series the AF transition occurs at lower temperatures than the MIT.

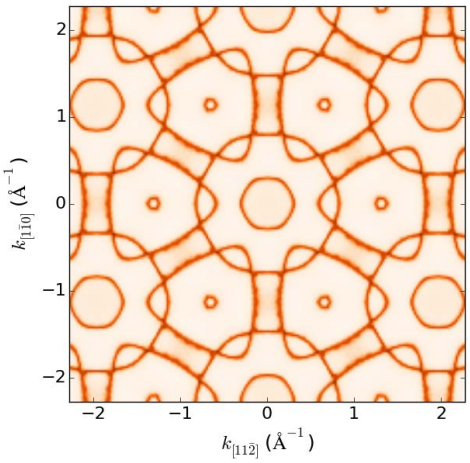

Figure 1: *Fermi surface of a $LaNiO_3$ film on $SrTiO_3$ substrate with 111 orientation.*

The goal of this project has been to understand the interplay between structural distortion, MIT, and magnetic order in rare earth nickelates, and to quantitatively describe trends across the series. Our work has solved the long-standing problem in the field of how to describe the electronic structure of these materials by focusing only on the low-energy e_g states and taking electronic correlations into account [11], has revealed the key interplay between Mott and Peierls-like physics, and has been verified experimentally in joint collaborations [12]. The effect of strain and of growing $\mathrm{LaNiO_3}$ in the [111] orientation was also studied (Fig. 1).

The methods development that we made as part of this project in the general framework for combined density functional theory (DFT) + dynamical mean-field theory (DMFT) calculations are all available within the TRIQS/DFTTools library [13].

Furthermore, the MARVEL theory-experiment collaboration on nickelates triggered an important achievement in terms of materials synthesis: the growth of single crystals by the group of Marisa Medarde at PSI (PP7 Sec. 3.1, p. 49).

3.2 DFT+DMFT study of strain and interface effects in d^1 and d^2 t_{2g} perovskites (Nicola Spaldin — ETHZ, Thorsten Schmitt — PSI)

The goal of this project has been to understand and predict the emerging properties of complex oxide thin films and heterostructures containing early transition metal perovskite oxides, such as, e.g., $LaTiO_3$, $LaVO_3$, or $CaVO_3$. Many of these materials are close to a Mott metal-insulator transition (MIT) and thus conventional density functional theory (DFT) is not suitable to describe these systems. We have therefore employed DFT in combination with dynamical mean-field theory (DFT+DMFT), a recently developed advanced electronic structure method suitable for the description of correlated electron systems both in the itinerant and localized regime.

We have shown that compressive epitaxial strain induces an insulator-to-metal transition in the bulk Mott insulator $LaTiO_3$ [152], but not in $LaVO_3$ [14], thereby explaining recent experimental observations [153]. Building on these results, we have then performed a systematic study of strain effects in early transition metal perovskites, allowing us to formulate a set of general rules regarding the effect of epitaxial strain in this class of materials [15].

One outcome of our systematic study is, that tensile epitaxial strain generally promotes Mott insulating behavior. Indeed, our calculations predict a MIT in otherwise metallic $CaVO_3$ for a tensile epitaxial strain of $\sim 3.5\%$. Our experimental collaborators at PSI (group of Thorsten Schmitt) are currently working on verifying our prediction (PP7 Sec. 3.3, p. 51). We have also identified a strong surface effect in oxide thin films , which tends to make the surface layer more correlated than the bulk material (Fig. 2).

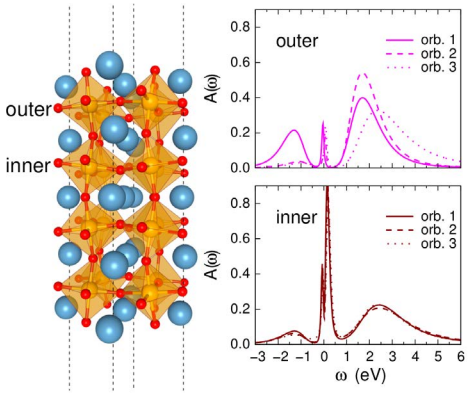

Figure 2: *Right: layer-resolved spectral functions for a free-standing 4-layer $CaVO_3$ slab (shown on the left). It can be seen that the electrons in the outer (surface) layer are strongly correlated, forming a very sharp quasiparticle peak around the Fermi level ($\omega = 0$). In contrast, the inner layer behaves nearly bulk-like.*

3.3 Multiferroics (Nicola Spaldin — ETHZ)

A goal of the MARVEL proposal was the rational design of new multiferroic materials. In this direction we have identified an entirely new mechanism for forming polar magnetic spirals and used this in collaboration with our experimental colleagues to generate new room-temperature multiferroics. The transition-metal oxide $YBaCuFeO_5$ was previously reported to have a magnetic spiral state of unknown origin. In addition, it was recently observed [154] that the transition temperature T_s to the magnetic spiral phase can be tuned from $T_s \sim 150$ K to $T_s \sim 300$ K by changing the annealing conditions after synthesis. Motivated by this observation, we used *ab initio* calculations to analyze the energetics of possible Cu^{2+}/Fe^{3+} occupational disorder [16] in $YBaCuFeO_5$ and extracted the relevant magnetic exchange couplings. We found that low-energy disordered states that frustrate the magnetic order exist (Fig. 3). Using Monte Carlo simulations for a model system with random impurities, we demonstrated the emergence of a magnetic spiral phase with properties (such as T_s and wave vector at low temperatures) dependent on the concentration of impurity bonds in qualitative agreement with the experimental observations on $YBaCuFeO_5$ [17, 18]. Our findings open a new mechanism for the design of high-temperature multiferroics.

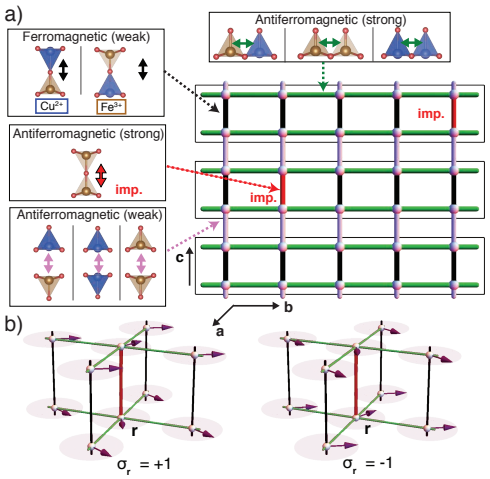

Figure 3: *(a) Nearest-neighbor exchanges and local frustrating impurity bonds (red lines) for the three dimensional model of $YBaCuFeO_5$. (b) The spin canting (clockwise or counter-clockwise) at an impurity bond can be encoded into an Ising variable.*

3.4 Exotic model Hamiltonians (Nicola Spaldin — ETHZ, Matthias Troyer — ETHZ, Thomas Schulthess — ETHZ, Dirk van der Marel — UniGE)

a) Ab initio *design of a new material whose Hamiltonian is that of the single-band Hubbard model* The "standard model" of condensed matter physics is widely regarded to be the Hubbard model. It augments independent-electron band theory through a single parameter to account for electron-electron correlations and has been remarkably successful at addressing a range of correlation effects in transition-metal materials. However, beyond one dimension the problem is intractable and so much current research aims at finding appropriate approximations for obtaining the Hubbard model phase diagram. In this project we explored a new approach: whether *ab initio* methods can be used to design a material whose Hamiltonian is exactly that of the Hubbard model so that its solution can be found by measuring the material properties. After identifying an appropriate crystal class and several appropriate chemistries, we used density functional theory and dynamical mean-field theory to screen for the desired electronic band structure and metal-insulator transition. We then explored the most promising candidates for structural stability and suitability for doping and propose specific materials for subsequent synthesis. Finally, we identified a regime — that should manifest in our bespoke material — in which the single-band Hubbard model on a triangular lattice exhibits exotic d-wave superconductivity [19].

b) *Higgs- and Goldstone modes in h-$RMnO_3$* The hexagonal rare earth manganites h-RMnO$_3$ undergo a symmetry-lowering phase transition from a high-symmetry paraelectric to a low-symmetry ferroelectric phase at around 1200 K. The free energy for the phase transition can be expanded in terms of a 2-dimensional order parameter (Q, Φ) corresponding to a K_3 phonon mode of the high-temperature structure, and a secondary order parameter P which gives the ferroelectric polarization [155]:

$$\begin{aligned} F = &\frac{a}{2}Q^2 + \frac{b}{4}Q^4 + \frac{Q^6}{6}(c + c'\cos 3\Phi) \\ &+ Q^3 P \cos 6\Phi + \frac{1}{2}Q^2P^2 + \frac{a_p}{2}P^2 \\ &+ \sum_{i=\{x,y,z\}} s_i \left[(\nabla Q)^2 + Q^2(\nabla\Phi)^2\right] \end{aligned} \tag{4.1}$$

This free energy has the form of a "Mexican hat" potential with six minima in the brim of the hat reflecting the symmetry of the system. A material described by such a potential has distinctive phonon modes corresponding to motion of the atoms around the brim of the hat (the Goldstone mode) and up and down the sides of the hat (the Higgs mode). In this project we have compared the behavior of these modes in two hexagonal manganites: ErMnO$_3$, in which the energy barriers between the minima in the brim of the hat are large, and InMnO$_3$, in which these barriers can be engineered to be negligible so that the Goldstone mode is close to zero frequency. In the latter case we identified, in collaboration with the group of Dirk van der Marel (UniGE), a renormalization of the Higgs mode due to anharmonic coupling.

3.5 Novel topological electronic phases (Matthias Troyer — ETHZ, Oleg Yazyev — EPFL)

The most prominent result in this direction was the discovery of the type-II Weyl fermions and their host materials — topological type-II Weyl semimetals [2]. Topologically protected crossings of two bands, called Weyl points, occur in these materials near the Fermi level, producing low energy excitations with linear dispersion. While standard (type-I) Weyl points have a point-like Fermi surface and result in low energy excitations that are the Weyl fermions of quantum field theory, the type-II Weyl points occur at the boundary between electron and hole pockets and realize excitations (Fig. 4) that are not present in relativistic theories due to the violation of Lorentz symmetry in condensed matter systems. These materials are expected to exhibit a range of novel physical effects, especially in magnetotransport. Finding candidate materials that realize this new topological phase was enabled by the hybrid Wannier function technique for calculating topological invariants implemented in the Z2PACK software package [20]. This package was developed in the group of Mathias Troyer in collab-

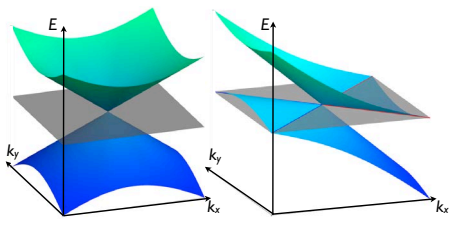

Figure 4: *Possible types of Weyl points. Left panel: type-I Weyl point with point-like Fermi surface. Right panel: type-II Weyl point is the touching point between electron and hole pockets [2].*

oration with the group of Oleg Yazyev. The type-II Weyl semimetal phase was predicted to exist in orthorhombic WTe_2 [2] and $MoTe_2$ [21] and some of the predictions were experimentally confirmed [10, 22]. Further search for novel topological electronic phases has led to the discovery of two new gapless phases that realize more complicated band degeneracies, namely the nodal chain metals [3] and the triple-point semimetal [9]. Candidate materials realizing these novel phases have been proposed.

3.6 High-throughput search for novel topological materials (Oleg Yazyev — EPFL, Matthias Troyer — ETHZ)

In order to realize systematic search for novel topological materials, we developed an automated computational protocol for the high-throughput screening of materials, outlined in Fig. 5. Our search relies on public databases of known materials, primarily the International Crystal Structure Database (ICSD). Initial prescreening is performed using simple criteria such as chemical composition, unit cell size, and crystallographic space group. The materials are then subject to first-principles electronic structure calculations based on density function theory performed using the QUANTUM-ESPRESSO package. The crucial step in identifying candidate materials is the calculation of respective topological invariants, which is achieved using the above-mentioned Z2PACK approach [20], which is especially suitable for high-throughput calculations. Finally, the information about candidate materials is passed to experimental collaborators in order to attempt experimental confirmation of theoretical predictions.

Following the initial prescreening, first-principles calculations of over 2'000 candidates materials from the ICSD database have been performed. Several promising candidates have been investigated in great detail. One important result is the discovery a new strong topological insulator, the quasi-1D bismuth iodide β-Bi_4I_4, which presents a number of properties not seen in other topological materials [4]. This material is characterized by a low concentration of intrinsic charge carriers and highly anisotropic surface-state Dirac fermions. Being a strong topological insulator with Z_2 indices (1;110), β-Bi_4I_4 is placed in proximity to two topological phase transitions, leading to a weak topological and trivial insulators. Most importantly, this work demonstrates the entire cycle of materials discovery starting from theoretical prediction to materials synthesis and photoemission experiments confirming the topological phase. This work also initiated broad theory-experiment exploration of new members of the family of quasi-1D bismuth halides.

Another successful example is the prediction of the robust type-II Weyl semimetal phase in diphoshpides MoP_2 and WP_2 [6]. These materials have 8 Weyl nodes, but the nodes of opposite chirality are well separated in momentum space. As a consequence, the Weyl semimetal phase in MoP_2 and WP_2 is expected to be very stable with respect to external perturbations, and should give rise to extended Fermi arc states easily observable experimentally. Furthermore, hidden Weyl points that are revealed by applying magnetic fields were discovered in $TaAs_2$ and $NbSb_2$ [23].

3.7 Topological properties of semiconductor nanostructures (Matthias Troyer — ETHZ)

Superconducting wires with topologically nontrivial band structure are actively considered as a platform for topological quantum computers [156, 157, 158]. The so-called Majorana zero modes at the end of these wires realize non-Abelian anyons and their braiding can be used to perform quantum computations. We aim at the search of optimal materials for topological nanowires and the development of accurate tight-binding models for the numerical simulations of realistic experimental setups used to produce and manipulate topological qubits.

A set of highly accurate symmetric tight-binding models was derived for several binary zincblende and wurzite compounds currently used in experiments on realizing Majorana fermions in quantum wires. These models were used to identify directions for the wire growth with maximal spin-splittings [24], necessary for inducing Majorana fermions, and to study the quantum spin Hall effect [159] in InAs/GaSb quantum wells. A combination of tight-binding modeling with fist-principles calculations allowed us to show that spin-splittings can be greatly enhanced in disordered compounds $InAs_xSb_{1-x}$ relative to the clean InAs and InSb. The same work identified a possible ordered phase of this compound for $x = 0.5$ as a material realizing several possible topological phases: topological insulator, topological semimetal of a new kind, and a semiconductor with spin-orbital splittings an order of magnitude larger than those in materials used in the current Majorana experiments [7]. The developed tight-binding mod-

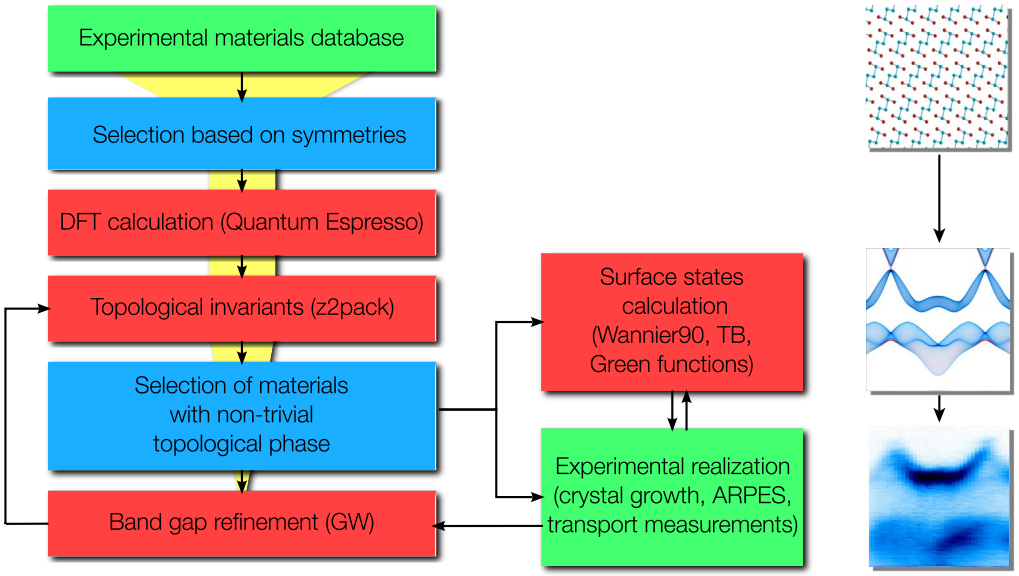

Figure 5: *Scheme of the workflow of high-throughput screening for novel topological materials. Panels on the right show the crystal structure, predicted and measured band dispersion for the discovered topological insulator β-Bi_4I_4 [4].*

els were also used to characterize topological effects in two-dimensional semiconductor heterostructures [25]
Finally, we developed a numerical method for calculating the topological contributions to the orbital magnetoelectric response in real materials [26]. We expect that the developed method will be used not only for topological materials, since it greatly facilitates the search for good magnetoelectric materials — a task of immediate technological importance.

4 Contribution to overall goals and initial proposal

VP1 has contributed directly to the overall goal of the NCCR of designing new materials with specific targeted functionalities in advance of their synthesis, notably the single-band Hubbard materials, candidate materials realizing topological insulator phases, as well as several new semimetallic topological phases that were not anticipated in the initial proposal. Some of our predictions already received experimental confirmation. The goals of high-throughput classification is largely attained by now. These achievements put us in the forefront of the materials discovery community oriented towards topological and strongly correlated materials.

5 Collaborative and interdisciplinary components

The work on topological materials is largely a result of close collaboration between the groups of Matthias Troyer (ETHZ) and Oleg Yazyev (EPFL). Collaboration with the group of Nicola Marzari (EPFL) has been instrumental for interfacing Z2PACK with the WANNIER90 software package [160]. In addition, several collaborations with experimental groups have been established. The PP7 project with the group of Ming Shi (PSI) dedicated to the experimental verification using angle-resolved photoemission spectroscopy (ARPES). First results addressing the Weyl semimetal phase in TaP have already been published [5], while another successful collaboration with experimentalists include the identification of topological insulator phase in $ZrTe_5$ [8, 27]. A collaboration with experimental groups in Copenhagen (C. Marcus and P. Krogstrup) on growing semiconductor nanowires for topological physics and experimentally verifying their properties is under way. We also collaborate with Microsoft Station Q (Santa Barbara) on semiconductor device simulations based on the tight-binding models derived here. The transition-metal oxides work has involved collaborations between Georges and Spaldin (DFT+DMFT), Spaldin, Troyer and Schulthess (single-band Hubbard model), and Spaldin and Troyer (magnetic spiral multiferroics) within VP1 as well as with multiple experimental groups (Medarde, van der Marel, Schmitt, Rüegg, Rossell) within PP7.

Vertical Project 2 VP2 — Novel Materials Applications

Project leaders: Ursula Röthlisberger (EPFL), Alfredo Pasquarello (EPFL)

Participating members: Ursula Röthlisberger (EPFL), Alfredo Pasquarello (EPFL), Jürg Hutter (UZH), Nicola Marzari (EPFL), Alessandro Curioni (IBM), Clémence Corminboeuf (EPFL), Daniele Passerone (Empa), Wanda Andreoni (EPFL)

Summary and highlights: The VP2 project is focusing on four grand-challenge problems, which consist in identifying optimal materials for solar cells, for water-splitting catalysts, and for solid-state ionic conductors. The fourth challenge consists in developing a platform for the discovery of low dimensional materials. Each of the research teams involves researchers from VP2, from the horizontal projects of MARVEL, and experimental partners. All projects are growing towards material searches on databases through the AiiDA platform (PP6). The scientific output achieved so far is impressive. However, the full potential of VP2 still lies ahead, as the synergies continue to grow and the material searches enter an operative phase.

1 Project overview

The ultimate goal of the VP2 project consists in identifying optimal materials for specific functionalities through a computational search. To achieve this goal, VP2 has gone through a dynamical transformation process by which synergetic research teams have been formed and specific target functionalities have been identified. VP2 has now naturally evolved to contain subprojects which deal with four grand-challenge problems: (1) materials for solar cells; (2) catalysts for water splitting; (3) solid-state ionic conductors; (4) low-dimensional materials. The first three projects target materials with specific functionalities, while subproject (4) focuses on the computational discovery of new low-dimensional materials, which could turn useful for various functionalities, as evidenced by the common interests between subprojects (2) and (4) within VP2, as well as by the collaborative effort between subproject (4) and VP1. To achieve this new organisation, many existing subprojects either have merged or have been discontinued, as for instance the project on CO_2 capture (Sec. 6).

As a result of this restructuring, each of the grand-challenge projects assembles several group leaders of VP2 within an organic collaboration which targets common objectives. Moreover, each of the projects also involves group leaders of the horizontal projects, through issues that concern methods (HP3) and/or sampling techniques (HP4). Remarkably, all the projects are getting ready for carrying out searches on databases through the AiiDA platform developed in PP6 and for using the machine learning principles developed in HP5. Further, it is worth highlighting that all projects involve experimental partners, which can thus challenge the computational results. The structure of MARVEL has turned out to be instrumental in promoting the interaction between all the scientists involved.

In the following, the various grand-challenge projects are described in detail. For each project, a summary of the first 33 months of MARVEL is provided. In addition to identifying the constituted research teams, particular emphasis is devoted to highlighting the specific goals, the achieved progress, and the future directions. In particular, the scientific outputs of VP2 already counts 79 publications, 11 of which have appeared in the prestigious series of the *Nature* Publishing Group and 2 in *Science*. It is expected that the present structure of VP2 ideally takes advantage of the available expertise offering a significant competitive potential to the VP2 grand-challenge teams compared to other efforts worldwide. The present organisation also constitutes an important asset for envisaging the research activity in phase 2.

2 Novel materials for solar cells

Ursula Röthlisberger — EPFL, Alfredo Pasquarello — EPFL, Stefan Goedecker (HP4) — UniBas, Michele Parrinello (HP4) — USI, Anatole von Lilienfeld (HP5) — UniBas, Expt.: Michael Grätzel — EPFL, Francesco Stellacci — EPFL

The overall goal of this subproject is to find new routes for the improvement of existing solar cell (SC) materials and to design new ones

using the tools of computational materials science. In particular, the subproject sets out to achieve an atomistic-level rationalization of the properties of SC materials, such as their stability, spectral characteristics, and transport properties. Three main types of SC materials are considered: (i) TiO_2-based dye-sensitized solar cells (DSSC), (ii) organic photovoltaics (OPV), and (iii) halide perovskites.

a) *Dye-sensitized solar cells (DSSC) and organic photovoltaics (OPV)* A systematic study to maximize the solar absorption of dye sensitizers has been carried out. The role of the molecular packing of the dyes on the TiO_2 surface was also addressed [28, 29]. This effort led to the rational molecular design of dyes for DSSC and to a new record in photoconversion efficiency [28]. In this context, a classical force-field for ruthenium-based and porphyrin-based systems has been developed [29]. This work involved a collaboration between the **Röthlisberger** group and the experimental groups of **Grätzel** and **Stellacci**. The studies of OPV systems have focussed on the characterisation of the charge transfer states in these materials and its relationship to the high quantum yields in OPVs [30].

b) *Halide perovskites* The study on photovoltaics based on halide perovskites has been carried out by the **Röthlisberger** group in close and continuous collaboration with the **Grätzel** group. For perovskites with the general formula ABX_3, the conducted research aimed at understanding the factors governing the stability, the electronic, and the transport properties of these materials, as a function of chemical composition, crystal structure and temperature. In particular, this research led to the design of new perovskite materials with enhanced thermal and chemical stability. In this framework, the stabilization mechanism of mixed-cation formamidinium/cesium (FA/Cs) lead iodide perovskites was identified [31], an explanation for the observed $J-V$ hysteresis in hybrid organic-inorganic perovskites has been suggested [32], and the temperature dependence of the photoluminescence spectra of $CH_3NH_3PbI_3$ ($MAPbI_3$) could be rationalized [33]. Importantly, correlations between electronic band edge positions and orbital overlap for B and X ions were unravelled and enabled a suggestion of new routes for the band gap tuning in halide perovskites [34]. This effort is at the origin of the collaboration between the **Röthlisberger** and **von Lilienfeld** groups, with the aim of developing improved searches based on combinations of genetic algorithm optimisations and machine learning models. Additionally, the **Röthlisberger** and **Pasquarello** groups started a joint project to generate reference data for band gaps through the self-consistent GW schemes developed in Sec. 3. These data would serve the purpose of validating training data used for the subsequent development of machine learning models in the **von Lilienfeld** group.

c) *Phase discovery and phase diagrams of halide perovskites* Due to the liquid processing of hybrid organic-inorganic lead halide perovskites, there is only limited control of the phase that is formed. This is a problem for halide perovskite systems, that exist in different phases [161]. Since the crystalline structure crucially affects the optical and transport properties, a complete knowledge of the stability ranges of the various crystalline phases is crucial for the design of suitable photovoltaic materials. In a collaborative effort, the **Röthlisberger** and **Parrinello** (HP4) groups are applying force-field based molecular dynamics simulations together with variational enhanced sampling techniques to study crystal growth and nucleation processes of these materials.

The exhaustive explorations of the phase space of crystals that are often characterized by energy barriers of hundreds of k_BT is computationally a highly demanding task. In a collaboration of the **Röthlisberger** and **Goedecker** (HP4) groups, the minima hopping (MH) method [162] has been employed to identify crystalline structures of $CsPbI_3$ as well as of $MAPbI_3$. Minima hopping is an efficient method to find the ground state as well as other low energy configurations of complex systems. It consists of a sequence of molecular dynamics escape moves followed by local geometry optimizations and exploits empirical relations such as the Bell-Evans-Polanyi principle, which links the height of a saddle point with the energy difference of the two minima that it connects. Using a feedback mechanism based on fingerprints, it is avoided that configurations are visited many times. The application of MH to identify the phases of a crystalline system requires an accurate model of the atomic forces. Density functional theory (DFT) has proven to work well for lead halide perovskites, with an error in the lattice parameters of only 1%. However DFT is computationally rather expensive, which makes it unsuitable for an extensive screening of the phase space of these materials. Therefore a classical force-field has also been used.

Several MH simulations were performed for

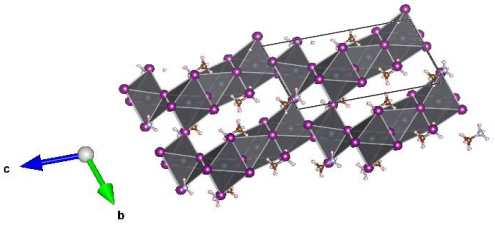

Figure 6: *One of the novel structures of $MAPbI_3$ obtained by MH simulations.*

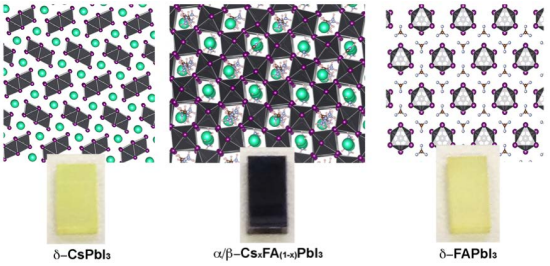

Figure 7: *Stabilisation of the mixed perovskite phase formed from two simple non-perovskite phases [31].*

$CsPbI_3$. In addition to the experimental δ phase and cubic perovskite phases, many other phases were discovered. In this case, the Quantum-ESPRESSO code was coupled with the minima hopping algorithm using a communication scheme based on sockets. All the structures have in common that they contain PbI_6 octahedra that share corners, edges, or faces. In the non-perovskite phases, each PbI_6 octahedron shares an edge and has three neighboring PbI_6 octahedra, whereas in the cubic phase the PbI_6 octahedra share all their six corners with neighboring PbI_6 octahedra. In addition, several MH simulations were performed for $MAPbI_3$. In this case, a fixed-point charge force-field has been used [163]. This model is able to describe some of the features of $MAPbI_3$, but it fails to capture the details of the transition from orthorhombic to tetragonal phase. However, in this way many crystalline structures as well as defect structures have been found (Fig. 6). These structures are currently examined further to understand the dynamics of these materials [35]. To overcome the limitations associated to the first generation polarizable force model developed for $MAPbI_3$, a force-matching technique is currently applied for the parametrization based on reference data from the first principles molecular dynamics. The new version of the polarizable force-field will also be used for the simulation of mixed cation perovskites with improved thermal and structural stability [31].

d) *Future work* The research is currently centered on establishing the factors governing the stability of the perovskite phase with respect to other competing crystal forms that are unsuitable for photovoltaic applications. It is one of the goals of this project to computationally identify ways to stabilize the perovskite phase at different temperatures using ionic mixing (substitution of A, B or X species, Fig. 7). The monovalent A-cation substitution route is currently being explored and a corresponding publication is being prepared. The same approach enables a simultaneous band gap tuning, that is also investigated in the present project. The studies on the substitution of B and X ions in ABX_3, in particular in view of lead-free compounds, are also under way. Future research will focus on the application of a multi-objective genetic algorithm toolbox developed within MARVEL to optimize the composition of mixed halide perovskite materials and will address electronic structure modulations in addition to the stability.

3 Superior electrocatalysts for the oxygen evolution reaction

Clémence Corminboeuf — EPFL, Jürg Hutter — UZH, Alfredo Pasquarello — EPFL, Nicola Marzari — EPFL, Joost VandeVondele (HP3) — ETHZ, Anatole von LilienFeld (HP5) — UniBas, Expt.: Xile Hu — EPFL, Greta Patzke — UZH, Thomas Schmidt — PSI, Christophe Copéret —ETHZ, Raffaella Buonsanti — EPFL

The research activity on water splitting has developed in two main directions: (i) the development of *tools* and *design principles* to screen the next generation of electrocatalysts for the oxygen evolution reaction (OER); this is a necessary step prior to the collaborative large scale screening of novel classes of *OER catalysts* using the *high-throughput* instrumentation and the 2D material database developed by the **Marzari** group; (ii) the examination and development of various electronic structure methods for the accurate description of the most relevant descriptors associated with both the catalysts and the photoanodes.

e) *Tools and design principles* One of the key strategies chosen to discover novel catalysts was to develop a unified perspective on catalysis through exploiting the paradigms of both homogeneous and heterogeneous catalysis. From the computational perspective, the identification of improved heterogeneous catalysis is essentially based on a pure thermodynamic picture and a global description of the

catalytic reaction cast into volcano-based plots, which permit facile comparison and screening of large numbers of potential candidates. On the other hand, the state-of-the-art of homogenous catalysis requires deep mechanistic insights (both intermediate and transition states) of the individual catalysts. The **Corminboeuf** group placed large efforts into combining these two paradigms as a way towards achieving novel generations of catalysts. Their specific objectives were twofold, (i) transferring the efficient screening tools derived for heterogeneous/electrocatalysis to molecular catalysts and (ii) increasing the complexity of heterogeneous catalysts and the underlying reaction mechanisms to break linear scaling relationships limiting the OER reaction.

To address the first aspect and with the perspective of identifying unique molecular catalysts for OER, the **Corminboeuf** group established the relevance of volcano plots for screening *homogeneous* catalysts. This effort was accomplished by considering prototypical homogeneous reactions [36, 37]. They then demonstrated that the predictive power of volcano plots could be increased through the inclusion of kinetic data [38], which often become essential in molecular catalysis. Together with PSI, the **Corminboeuf** and **Hutter** groups are now using this tool to analyse molecular catalysts for water splitting. The current focus is on Co-pyridine and -porphyrine-based molecules as well as Co(II)-based cubanes (Fig. 8), which are currently the most promising mimics for nature's extremely efficient water oxydation catalysts. Derivatives of molecular systems such as $[Co_4^{II}(hmp)_4(\mu\text{-}OAc)_2(\mu_2\text{-}OAc)_2(H_2O)_2]$ (hmp = 2-(hydroxymethyl)pyridine) and $[Co_3^{II}Er(hmp)_4(OAc)_5H_2O]$ are ideally suited for this screening thanks to the insights gained from detailed atomistic studies performed in the **Hutter** group [39, 40, 41, 42, 43, 44, 45][164].

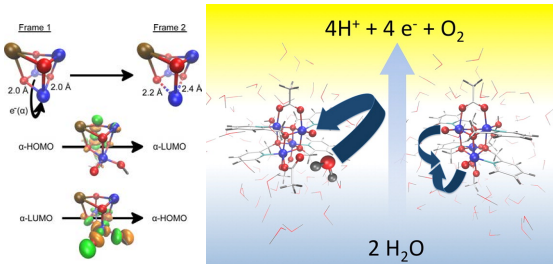

Figure 8: *Water oxydation by Co cubanes. Changes in the cubane cage and electronic structure between two different frames of a NEB pathway describing the water attack on 2-Tm and frontier orbitals of the first frame are shown.*

Those investigations, performed in collaboration with the experimental group of **Patzke** (UZH), identified existing correlations between the catalytic activty and the nature of the ligand [39, 40] and other crucial structural and electronic motifs [41, 42]. Finally, the screening strategy of homogenous catalysts elaborated by the **Corminboeuf** group also initiated a novel collaborative effort with the **von Lilienfeld** group. The two teams are currently building a machine learning model that could dramatically reduce the computational time associated with the construction of volcano plots.

The second task consists in borrowing the tactics in homogenous and enzyme catalysis to overcome the limitations inherent to the OER. The latter reaction suffers from considerable overpotential, arising from the universal scaling relation between the binding energies of the various surface-bound intermediates. Recently, the **Corminboeuf** group was able to break these linear scaling relationships through avoiding the formation of the energetically costly intermediates via a different mechanism [46]. The proposed strategy was validated experimentally by the **Hu** group (EPFL), who discovered a bifunctional catalyst that performs two orders of magnitude better than the current state-of-the-art. The proposed mechanism and associated descriptor are currently being used to screen the portfolio of 5'600 layered materials extracted from crystallographic databases by the **Marzari** group (Sec. 5). Such screening is expected to yield unprecedented catalysts that are more efficient. Using the same design principle and exploiting the same mechanism, the **Hutter** and **Corminboeuf** groups are also trying to identify novel molecular-based catalysts, which offer a unique opportunity for easy fine-tuning and multifunctionalization. Along the same line, the screening of the rare earth lanthanide perovskites, such as those investigated in the **Marzari** group, constitutes an appealing class of materials featuring multifunctional active sites.

f) *Accurate electronic structure description* The above studies relied upon relatively crude computational static model systems excluding the presence of explicit solvent molecules. Within the perspective of improving the models and investigating (photo)catalytic processes in the presence of the water solvent, the **Pasquarello** group has searched for an optimal functional to describe the electronic properties of water, such as the band-edge levels and relevant redox levels. They first focussed on

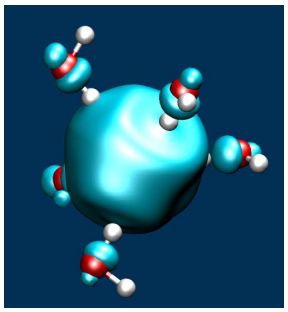

Figure 9: *Isodensity of the majority fivefold coordinated hydrated electron as obtained with hybrid-vdW simulations. The isodensity contour encompasses 60% of the charge density of the hydrated electron.*

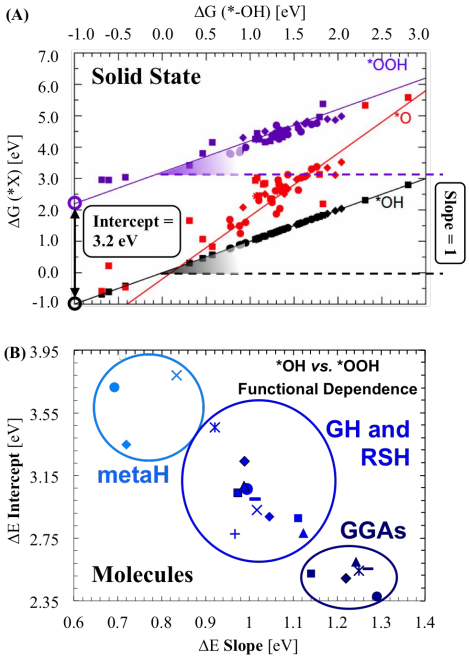

Figure 10: *(a) Typical DFT linear scaling relationships for heterogeneous electrocatalysts of the oxygen evolution reaction (OER). The Gibbs free energies are relative to the hydroxo intermediate (*OH). For the solid state computations, the slope and the intercept of the linear regression are found to be independent from the density functional used. (b) Molecular electrocatalysts of the OER: strong dependence of the intercepts and slopes on the density functional used for the computation. Three distinct regions comprise the results from the GGAs, the global and range-separated hybrids (GH and RSH) and the meta-hybrid functionals (to be published).*

the description of structural properties of liquid water by considering the effect of van der Waals (vdW) interactions [47]. The approach was able to reproduce the experimental density in isobaric-isoenthalpic molecular dynamics simulations and to achieve an overall improved structural description with respect to a plain semilocal scheme. The vdW interactions are found to favor more compact structural motifs. In particular, in a joint collaboration between the **Hutter** and **Pasquarello** groups, it was verified that two important codes such CP2K and Quantum-ESPRESSO yield equivalent results [48]. To achieve a band gap in accord with experiment, they then developed a hybrid functional augmented by vdW interactions [49]. The redox levels in aqueous solution were studied through a combination of *ab initio* molecular dynamics and thermodynamic integration [50, 49]. In particular, they considered the H^+/H_2 level that defines the standard hydrogen electrode and sets a reference for direct comparisons with experiment. The agreement with experiment is very good for both band edge levels and redox levels [50, 49]. To further benchmark the functional, the electronic levels of the hydrated electron were addressed (Fig. 9) and found to be in very good agreement with experiment.

The accurate description of molecular systems, e.g. the Co-Cubanes, is also highly tricky since it necessitates the use of highly correlated methods (DMRG, FCIQMC). Efforts along this line are ongoing between the **Hutter**, Reiher (ETHZ) and Alavi (MPI Stuttgart) groups. These molecular benchmarks are especially relevant to the volcano-based screening of molecular catalysts, which relies upon achieving accurate linear scaling relationships (Fig. 10).

In addition to having efficient catalysts, focus should also be placed on the joint discovery of inexpensive photoanode materials that could harvest the sunlight and open new horizons for low-cost solar cell production. This on-going search strongly benefits from recent theoretical progresses that allow for accurate computation of band gaps by the **Pasquarello** group. The team developed a self-consistent GW scheme which accounts for vertex interactions and produces excellent agreement with experiment [51, 52, 53]. The electronic structure of liquid water could successfully be described by applying this scheme to configurations achieved with path-integral molecular dynamics [54]. In collaboration with the **Marzari** group, the same configurations are now used to confront the results with those of a Koopmans-compliant functional. The method is further being applied to more complex metal-oxides, such as $BiVO_4$ and Cu-V-O systems, that are proposed as photoanodes for water splitting (in collaboration with the experimental group of **Buonsanti**) and to halide perovskites (Sec. 2).

4 A search for solid-state ionic conductors

Alessandro Curioni — IBM, Nicola Marzari — EPFL, Berend Smit (HP4) — EPFL, Michele Ceriotti (HP5) — EPFL, Anatole von Lilienfeld (HP5) — UniBas, Expt.: Daniele Pergolesi (PP7) — PSI

Liquid organic electrolytes used in today's batteries are unreliable and inherently dangerous [165]. This project is close to finalizing a high-throughput (HT) screening procedure to search for new solid-state ionic conductors, thus providing candidate materials for next-generation batteries. A *detailed analysis* with first-principles (FP) techniques revealed the importance of strain and ion-ion correlations in fast-ionic conductors [55, 56] and led to the understanding of several mobility *descriptors* [166]; an *efficient modeling* based on our novel *pinball model* (PM) and new polarizable force-fields (p-FF), will be used in transport *simulations*; the *computational framework* was developed in the past three years and made publicly available to the MARVEL community as part of the AiiDA platform. This work already led to the prediction of a new family of solid state electrolyte materials [57].

g) *Analysis of selected materials* The **Curioni** group investigated the role of ion-ion correlations in two different materials. In $Li_7La_3Zr_2O_{12}$ (LLZO), the conduction mechanisms in two different structural phases were analyzed. It was described how the correlated motion in the tetragonal phase is replaced by single-event based conduction in the cubic phase [58]. In $Li_{10}GeP_2S_{12}$ [167], the centre of mass motion of correlated carriers was compared with the single particle behavior. It was observed that diffusion is highly underestimated when using the approximate Nernst-Einstein equation, due to a high Haven ratio. As an alternative class of materials, proton-conducting perovskites were investigated, in which a Grotthus-like transport mechanism is active. In collaboration with the experimental group of **Pergolesi** (PSI), the **Curioni** group was able to reproduce, for the first time, proton trapping and analyze strain to limit its effect.

h) *Descriptor search and modeling* Efficient HT screening requires a multilevel approach. For a preliminary selection of candidate structured from large datasets, the descriptors are based on static properties. One approach uses the Voronoi tessellation of structures to detect potential conducting pathways. This idea was expanded to include information on the time evolution of Voronoi cells in short molecular dynamics (MD) simulation. In another approach, the **Marzari** and the **Smit** (HP4) groups worked together and introduced potential descriptors based on the persistent homology and other topological features of materials.

The second step of the screening procedure requires a more detailed analysis of the dynamical properties. A kinetic Monte Carlo (kMC) approach, based on the automatic detection of diffusion network and the parametrization of barriers between its nodes, was first investigated. Despite promising results, it has become clear that kMC is only providing a limited amount of information at the cost of a very complex and expensive parametrization. Motivated by these difficulties, it was decided to investigate alternative approaches based on MD. One of the developed approaches is the novel PM, based on the hypothesis that cations in solid-state electrolytes move fully ionized in a relatively rigid energy landscape. At a first level of approximation, the position of the non-diffusive sublattice is fixed and the approach validated against FPMD simulations with similar constraints in the thio-LISICON family. It was then understood that charge transfer effects are crucial when describing the energy landscape, and this led to a significant improvement of our model (Fig. 11). P-FFs driven MD have already shown good results in reproducing both the structural parameters and the conductivity of LLZO [168]. However, their developments is highly affected by 30 years old methodologies, parameterizations, and transferability issues. The improvements and experience collected on automatic generation of

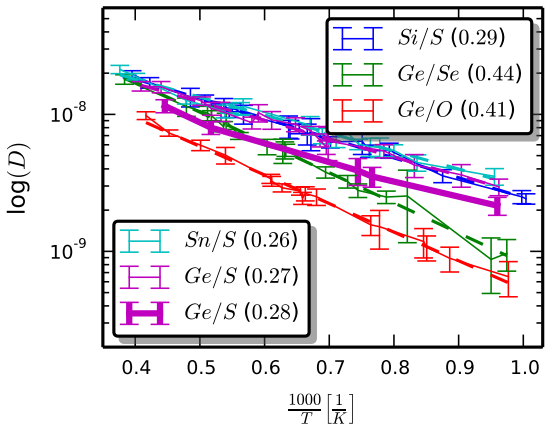

Figure 11: *Arrhenius behavior and activation barriers to diffusion (in brackets in eV) for structures of the thio-LISICON family ($Li_{20}A_2P_4B_{24}$, short A/B). One case ($Li_{20}Ge_2P_4S_{24}$) can be compared with the DFT result (thick line) and results are in excellent agreement (0.27 eV vs 0.28 eV).*

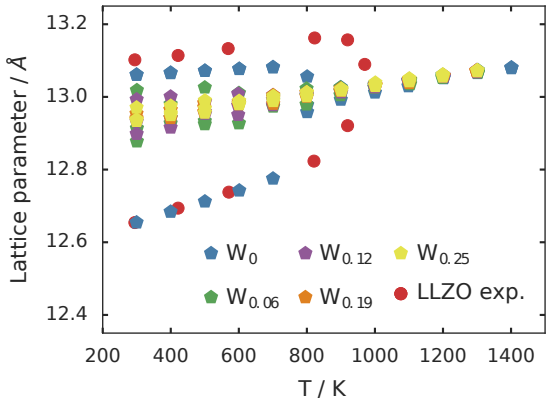

Figure 12: *Phase diagram of LLZO for W-doped structures. Stability of the cubic phase is enhanced by higher dopant concentration.*

parameters in the last years allowed the **Curioni** group to develop a robust methodology to parametrize polarizable potentials from FP and empirical data. Through the study of the dependency of the p-FF on its parameters, a strong dependency of the conductivity on the atomic polarizabilities was observed. Therefore, the efficient and reliable parametrization of p-FFs requires both classical forces minimization performed on experimental crystallographic structures and fitting of p-FF shell parameters to FP quantities. The accuracy of this method was assessed for undoped and W-doped garnet-type electrolytes. Not only is the present p-FF able to reproduce the transition of the structure between its cubic and tetragonal phase, but it can also successfully stabilize the cubic phase of the doped structure (Fig. 12). All these results have been presented in several conferences and have been submitted for publication.

i) *Computational framework* The **Marzari** group has implemented the PM in QUANTUM-ESPRESSO [169] and interfaced it with the AiiDA framework [59]. A channel analysis algorithm based on Voro++ [170] was developed to detect conduction paths in equilibrium structures. It was first intended to find conduction networks for our kMC approach but is also applicable as a diagnostic tool for conductivity. Furthermore, the **Marzari** group is continuing the analysis of the influence of thermostat and sampling technique on diffusion properties in collaboration with the **Ceriotti** group. All the acquired knowhow has then been transferred to the open-source MDWorkflow, a plugin to AiiDA that enables one to run MD simulations in an automated fashion. Additionally, the **Curioni** group has integrated the current developments with the activities of the **von Lilienfeld** group (HP5) to achieve the design of a new material discovery platform. The potential of this approach was demonstrated in the design of a new class of ionic conductor materials based on sodium oxoferrate, for which the joint effort was able to identify structures displaying promising ionic networks (channels). In particular, using data analytics and DFT calculations, the **Curioni** group identified atomic substitutions at the iron centers leading to higher Na ion conductivities. This initial effort has led to the filing of a patent [57] for novel ionic conductors.

j) *Future work* This project has led to the development of several promising methodologies for the search and the characterization of new ionic conductors that perform well for the families of compounds investigated so far (LLZO and LGPS). In the next phase, it is important to demonstrate their transferability to other material classes and assess their screening capabilities. Furthermore, these new techniques will be further elaborated in order to improve their predictive power and to exploit their full potential.

5 AiiDA-based discovery of low-dimensional materials and nanostructures

Nicola Marzari — EPFL, Daniele Passerone — Empa, Clémence Corminboeuf — EPFL, Jürg Hutter (HP3) — UZH, Oleg Yazyev (VP1) — EPFL, Michele Ceriotti (HP5) — EPFL, Expt.: Empa

The outstanding interest in low-dimensional structures in the past decades has been triggered by the discovery of a few compounds with exceptional properties: zero-dimensional (0D) fullerenes and quantum dots, one-dimensional (1D) carbon and boron nitride nanotubes, and, more recently, two-dimensional (2D) graphene, transition metal dichalcogenides and black phosphorus. Nonetheless these materials are nothing but the tip of the iceberg of a wealth of low-dimensional structures that can be engineered. In the first phase of MARVEL a major effort has been put in place to accelerate the discovery of novel low-dimensional materials and nanostructures through accurate first-principles simulations assisted by the AiiDA informatics infrastructure for materials [59]. Two main directions have been pursued: filling the knowledge gap on 2D materials, and designing 1D nanostructures with specific electronic properties.
Two-dimensional materials provide novel opportunities to venture into largely unexplored

regions of the materials properties space. Through high-throughput computational exfoliation of experimentally known compounds, the **Marzari** group has identified an extensive database of 1'844 exfoliable 2D materials [60] that will be made available online on the Materials Cloud portal (open spring 2017) and will be further investigated to disclose exceptional electronic, optical, magnetic, topological, and chemical properties.

The team started from a set of bulk 3D crystal structures extracted from the ICSD [171] and COD [172] databases with respectively 177'343 and 351'589 entries. The focus was set on experimentally-determined structures containing at most 6 different species amounting to 186'282 CIF files being initially retrieved using routines developed within AiiDA. A geometrical algorithm was conceived to identify potentially layered materials and was found to be generally sufficient to recognize low-dimensional units independently of their crystallographic orientation, dimensionality, and environment. The ensuing list of 5'619 layered materials has then been tested against accurate, validated van der Waals density functional theory simulations of the binding energies using two exchange correlation functionals: rVV10 [173] and vdw-DF2-C09 [174]. Over 3'200 unique layered structures have been relaxed and more than 2'600 binding energies have been computed. Compounds with sufficiently small binding energies and where dispersion relations affect interlayer distances are deemed exfoliable (Fig. 13). The 2D materials identified are in particular classified into groups of easily (1'053) or potentially (791) exfoliable compounds, showing that only a tiny fraction of possible 2D materials has been considered up to now. All 2D materials that are commonly exfoliated in experiments have been identified (Fig. 13), validating the approach. The enormous amount of calculations and results (over 3.7 million core hours) can be fully reproduced thanks to the deployment of AiiDA.

This extensive database provides a gold mine for future investigations and collaborations within MARVEL. The **Marzari** group has already started to screen for magnetic materials (with 112 magnetic insulators found) and topological insulators, and has computed the elastic constants of almost 700 layered materials. In collaboration with the **Corminboeuf** group they will search for novel 2D materials for efficient water splitting, while with **Yazyev** group (VP1) these 2D structures will be inspected to host the emergent physics of the Kitaev model.

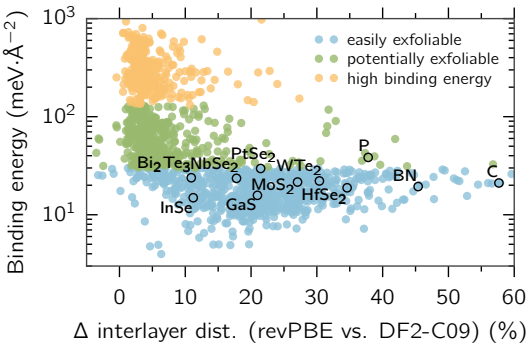

Figure 13: *1'844 novel 2D materials have been identified in this project (blue and green). Here, we show the binding energy vs change in interlayer distance predicted by vdW (DF2-C09) or non-vdW (revPBE) functionals, as classifiers of exfoliability. Well-known 2D materials are highlighted in the plot.*

The sketch-map tool developed by the **Ceriotti** group (HP5) will be applied to identify trends and prototypes in 2D structures, while the list of layered materials will represent a benchmark suite for RPA calculations performed in the **Hutter** group (HP3).

The 2D compounds identified can also serve as a basis for engineering 1D nanoribbons, 1D/2D bottom-up nanostructures and nanojunctions, with a wealth of potential applications. In this respect, a major effort has been set up in the **Passerone** group to study the possibility to tune the electronic properties of 1D carbon based heterojunctions by means of atomically precise doping. This has been done in close collaboration with **Empa**'s experimental facilities, that can provide atomically precise carbon based nanostructures. As a first step, the scanning tunneling spectroscopy (STS) simulation strategies were consolidated, for surface supported graphene based nanomaterials [61] and in the theoretical rationalization of the microscopy and spectroscopy measurements of different nanostructures [62, 63, 64, 65, 66, 67] [175]. In a second step, the electronic and optical properties of carbon based nanoribbons were screened, identifying the best candidates for photovoltaics applications. Preliminary exploratory work in this direction resulted in a collaboration between the groups of **Passerone** and **Curioni** with the delivery of new tools within the AiiDA framework managed by the **Marzari** group.

In a later stage, new frameworks were designed, to provide all the necessary tools for reliable high-throughput screening and engineering of low-dimensional structures. In particular, the **Passerone** group released a beta version of the AiiDA plugin for CP2K and developed an AiiDA workflow for band-

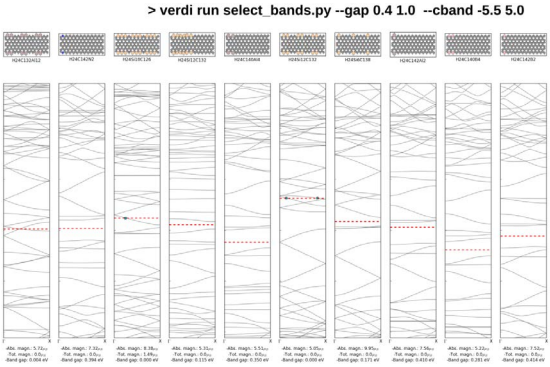

Figure 14: *Querying the AiiDA database for nanostructures with prescribed band gap characteristics.*

structure based screening in 1D nanostructures (Fig. 14). The workflow, which also parses spectroscopy data, will be released soon. The **Passerone** group also started populating a database of electronic properties of nanoribbons with atomically precise doping and tested the approach proposed by the **Curioni** group to access the optical properties of nanoribbons synthesized at Empa. Then, the **Passerone** group collaborated with the **Hutter** group (HP3) to test intensively the GW approach implemented in CP2K for finite size nanoribbons. The corresponding software developments will be merged into AiiDA, through a collaborative effort between the groups of **Passerone** and **Marzari** (PP6). In addition, a user-friendly web interface on the Materials Cloud is in the process of being designed and would allow experimentalists at **Empa** to compute and search properties of nanomaterials before synthesis. Also for the 1D nanostructures, a collaboration between the groups of **Passerone** and **Ceriotti** (HP5) has been started to explore the use of sketch-map tool and machine learning for this class of systems.

The recent experimental achievements at **Empa** in the direction of device demonstrators provide a strong motivation to extend the concepts already accessible to the AiiDA workflow that are being tested. Therefore, thanks to the theoretical screening of bottom-up synthesis from molecular precursors, and with a strong interplay with the discovery of novel 2D materials mentioned above, the following targets have been set within this project: 1) one- and two-dimensional bottom-up nanostructures and nanojunctions with applications in photovoltaics, thermoelectrics and water splitting; 2) devices based on exfoliated and bottom-up materials for applications in nanoelectronics; 3) porphyrin-based organic nanostructures with sensor applications; 4) complex materials based on the interaction between bottom-up and exfoliated low-dimensional units. These targets will be accompanied by several other activities on low-dimensional materials, ranging from unveiling the microscopic mechanisms underlying thermal transport in 2D [68, 69, 70] to the emergence of 1D metallic wires at polar discontinuities [71, 72], and to the multiscale computation of arsenene and antimonene transistor performance [73].

6 The industrial way for post-combustion capture of CO_2: optimizing the solvent

Wanda Andreoni — EPFL

Post-combustion carbon capture mainly employs solvent wet scrubbing, primarily using alkanolamine aqueous solutions as chemical absorbents. The prototype and most frequently used is mono-ethanolamine (MEA). The need for more efficient solvents has promoted a widespread empirical effort for the optimization of the solvent and of process-related parameters. Using DFT-based molecular dynamics, accelerated by metadynamics strategies, the **Andreoni** group has characterized the chemical reactions involved in both the uptake of CO_2 via absorption — in the form of either carbamate or bicarbonate — and its release leading to the amine regeneration. The resulting understanding of the corresponding mechanisms and of the role of diverse physicochemical factors is expected to be useful for the screening of possible solvents.

Using their expertise on MEA [176, 177, 178], the **Andreoni** group carried out a thorough comparison with other primary amines, namely MEA-derivatives (AMPD [74], AMP), a ring amine (BZA) and ammonia itself. The following unprecedented scenario is revealed. In all cases, the role of water — strongly underestimated in all previous approaches [75] — is essential to facilitate the development of the reactions. The amine-water interaction also differentiates MEA from its derivatives. Through the hydrophobic groups of MEA, the access of water molecules is limited and the probability of carbamate formation decreases. Moreover, the missed observation of the carbamate in AMP could be related to the improbable formation of the zwitterion. In AMP, the bicarbonate formation is the only path available for the capture of CO_2, despite the high free-energy barriers. In other amines, the formation of the zwitterion is essential not only for the formation of carbamate and carbamic acid, but also for the release of CO_2.

Horizontal Project 3 HP3 — Advanced Quantum Simulations

Project leader: Jürg Hutter (UZH)

Participating members: Jürg Hutter (UZH), Philipp Werner (UniFR), Mattias Troyer (ETHZ), Stefan Goedecker (UniBas), Nicola Marzari (EPFL), Joost VandeVondele (ETHZ)

Summary and highlights: We developed efficient continuous-time quantum Monte Carlo methods for correlated lattice fermions and designed an approach to compute fidelity susceptibility for correlated materials. A consistent GW+DMFT scheme which treats different orbitals with an appropriate level of accuracy was developed and implemented. We enabled simulations of electrochemical processes using MP2 and RPA and simulated aqueous redox systems by molecular dynamics and Monte Carlo using these methods.

1 Main goals and achievements

1.1 Main goals

Predictive quantum many-body simulations play a crucial role in materials science. The simulation software translates physical concepts into algorithms via models. The efficient implementation of the algorithms allow then the study of properties of new materials using high-performance computing platforms. By providing novel and improved simulation models, the HP3 subprojects work as enablers for the application projects in VP1 and VP2, and build a base for the techniques developed in HP4 and HP5.

1.2 Dynamical mean-field based methods

A first subproject is concerned with the description of strongly correlated systems and relies mainly on the dynamical mean-field method (DMFT). Within MARVEL, the Troyer and Werner groups have developed efficient continuous-time quantum Monte Carlo methods (LCT-QMC) [76, 77] and new algorithms to substantially reduce the sign problem [78]. They developed a fully parameter-free *ab initio* simulation method for correlated materials based on the GW+DMFT scheme. Their scheme extends previous efforts to realistic multi-band materials [79]. First applications to the cubic perovskite $SrVO_3$, a prototype strongly correlated metal with pronounced Hubbard bands [179, 180], showed that the standard interpretation has to be reconsidered. Non-equilibrium extensions to DMFT have been successfully implemented based on two complementary Floquet schemes.

1.3 Density functional theory and beyond

Methods that are going beyond the standard local density approach within the Kohn-Sham method are needed for many modern materials developments. Especially materials used in electro-catalysis need these improved methods even for a qualitative correct description of the basic principles and properties.

a) *Koopmans-compliant functionals* The Marzari group successfully further development Koopmans-compliant (KC) functionals [181][80] in orbital-dependent DFT. Enforcing the condition of Koopmans' compliance leads to orbital energies that can be interpreted as the quasiparticle excitations measured in photoemission experiments [81]. The concept has 4been applied to the band gap of liquid water [182] and DNA and RNA nucleobases with results in excellent agreement with experimental data [82].

b) *MP2, RPA, and G_0W_0 methods* Enabling simulations of electrochemical processes at the many-body correlation energy level using efficient algorithms for second-order Møller-Plesset perturbation theory (MP2) [83], the random phase approximation (RPA) [84, 85], and G_0W_0 approximation [86] have been the focus of the VandeVondele and Hutter groups. Applications to liquid water [87, 88] and aqueous redox systems [89] by *ab initio* molecular dynamics (MD) and Monte Carlo (MC) sampling were performed.

c) *Continuum solvation models* The Goedecker and Marzari group further developed the concept of self-consistent continuum solvation (SCCS) models [183]. The SCCS model was extended to the calculation of optical spectra [90] and it was coupled

with various periodic boundary correction schemes [91]. A novel solver for the generalized Poisson equation was developed and extended to the solution of the Poisson-Boltzmann problem [92]. The resulting scheme shows impressive performances and allows the modeling of systems in the presence of an applied electrochemical potential.

1.4 High-performance computing

The methods and algorithms developed in HP3 are implemented in the respective computer programs maintained by the individual groups. The programs and libraries ALPS, TRIQS, Quantum-ESPRESSO, CP2K, and BIGDFT are constantly updated and improved to allow for optimal usage of the high-performance hardware available in Switzerland. Recent scaling and performance results for CP2K were published in [84, 86, 85].

2 Scientific outputs

2.1 Publications and presentations

The scientific progress of the HP3 project has been documented in about 45 peer-reviewed publications. The main part of these highly technical, theory and algorithm centric reports is published in the leading international topical journals, e.g. *Physical Review* journals, *The Journal of Chemical Physics* or *Journal of Chemical Theory and Computation*. The work of HP3 has been presented at many conferences through invited talks, e.g. at Psi-k 2015, San Sebastian, or the annual conferences of APS and ACS. Numerous contributed talks and posters have been given by the doctoral students and postdocs at national and international conferences.

2.2 Prizes

Matthias Troyer has been awarded the 2016 Aneesur Rahman Prize for Computational Physics of the American Physical Society for his work on numerical simulations of quantum systems.

3 Progress of the different efforts

3.1 Troyer group

Our group aims at improving fermionic simulation methods with focus on negative sign problem and suboptimal scalings of the algorithms; at exploring usage of quantum information measures in material science research and to design and develop efficient and powerful fermionic simulation algorithms to facilitate material discovery. We developed efficient continuous-time quantum Monte Carlo methods (LCT-QMC) [76, 77] suitable for studying low-temperature phases of strongly correlated lattice fermions. These methods are free from time-discretization error and enjoy many flexibilities of the continuous-time QMC framework [184]. Combined with a newly discovered design principle of sign-problem free fermionic QMC methods [93], we mapped out the phase diagram of asymmetric Hubbard model [94] using LCT-QMC method. These results bridge the known limiting cases of SU(2) symmetric Hubbard model and the Falicov-Kimball model that is relevant to rare earth compounds. We systematically investigated the dependence of average sign on the choice of single-particle basis in the context of quantum cluster problems. We found out the sign problem can be substantially reduced by using a non-trivial single-particle basis which diagonalizes a subset of the intra-cluster hoppings [78]. This discovery has broad implication for cluster dynamical mean-field theory (DMFT) studies of multi-orbital systems and low-dimensional Hubbard models.

We developed a simple, efficient and generic approach to compute an important quantum information concept, fidelity susceptibility using quantum Monte Carlo methods [95]. It provides a fresh look at quantum phases and phase transitions going beyond the conventional Ginzburg-Landau paradigm. Based on this approach, we laid out the conceptual and technical foundation of investigating impurity quantum phase transitions and crossovers using fidelity susceptibility [96].

Constrained random phase approximation (cRPA) is one of the popular downfolding schemes to derive low-energy effective Hamiltonian of multi-orbital systems. We examined its reliability in [97] and found that the violation of the Pauli principle in the cRPA leads to overscreening effects when the interorbital interaction is small. This problem can be overcome by using a variant of the cRPA method which restores the Pauli principle.

Finally, we implemented an interface between our implementation of the density matrix renormalization group (DMRG) algorithm and quantum chemistry packages to provide an optimized and modern DMRG code for full-configuration-interaction calculations in chemistry [1].

3.2 Werner and Marzari groups

a) *GW+DMFT* We are developing a parameter-free simulation method for correlated materials. The approach is based on the GW+DMFT scheme [185]. Up to now, self-consistent GW+DMFT calculations have been implemented only for simple one-band models [186, 187] [98]. Our multi-tier approach for realistic multi-band materials is illustrated schematically in Fig. 15. Starting from a density functional theory calculation for the full range of bands in the solid, we first perform a one-shot GW calculation (G_0W_0). We then define an intermediate subspace I, for which the goal is to construct an accurate low-energy model. Furthermore, we introduce a possibly smaller correlated orbital subspace C, whose effective local interactions are treated by means of an impurity construction within an extended DMFT approach similar to [98]. Apart from the definition of the subspaces, there are *no free parameters* in this *ab initio* simulation approach, and there is *no double counting* of energies, as in standard LDA+DMFT.

In [79] we applied this consistent GW+DMFT scheme to the cubic perovskite $SrVO_3$, choosing the t_{2g} subspace for both I (tier II) and C (tier I). $SrVO_3$ has been considered a prototype strongly correlated metal, with pronounced Hubbard bands [179, 180]. Our calculations showed that this interpretation has to be reconsidered, and this is also confirmed by the recent extension of DFT+U by the Marzari group to DFT+U(ω).

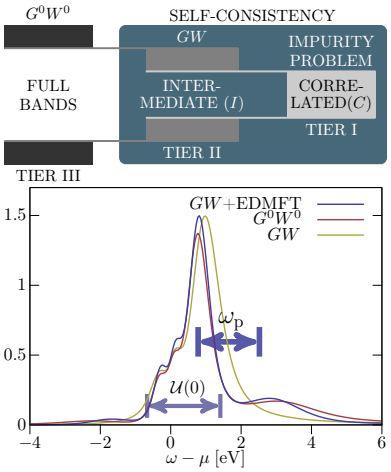

Figure 15: *Top: different levels of approximation in the multi-tier GW+DMFT scheme: The LDA+G_0W_0 treatment of the full range of bands (tier III) is used to construct the effective model for the intermediate energy space of Wannier functions (tier II), which is handled in GW. The local part of tier II defines the DMFT impurity problem (tier I). Bottom: local d-electron spectral function of $SrVO_3$ obtained using the GW+DMFT, G_0W_0, and self-consistent GW approximations. The static impurity interaction $U(0)$ is too small to produce Hubbard bands. Instead, the satellites are of a plasmonic origin.*

b) *Floquet+DMFT* The non-equilibrium extension of dynamical mean-field theory (DMFT) has recently emerged as a versatile tool for the study of non-equilibrium phenomena in correlated lattice models [188]. The goal is to develop a non-equilibrium DMFT based simulation approach for periodically driven solids. By employing a Floquet representation of the Green's functions enables the study of non-equilibrium steady states in driven-dissipative systems. We will apply this approach to the basic models for correlated electron and electron-phonon systems, and try to develop strategies for the non-equilibrium control of material properties. We have successfully implemented two complementary Floquet+DMFT schemes. The first scheme is aimed at the study of electron-phonon systems and employs the Migdal approximation as an impurity solver. It directly simulates the long-time steady-state which is reached in the presence of external driving, provided that the system is coupled to a (fermionic or bosonic) heat bath (Fig. 16a). We have applied this scheme to periodically driven superconducting states of the Holstein model, where the driving was implemented as a periodic modulation of the phonon potential. As shown in Fig. 16b, the effect of this driving is to weaken the superconductivity. The second Floquet+DMFT scheme employs a strong-coupling perturbative impurity solver and is aimed at the study of Mott insulating compounds and multi-orbital physics. We are currently using it to investigate the

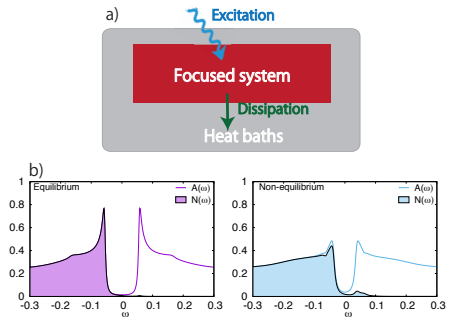

Figure 16: *(a) Illustration of the energy flow in a driven-dissipative system with coupling to heat baths. (b) Spectral function $A(\omega)$ and occupied states $N(\omega)$ of a superconducting Holstein model in equilibrium (pink) and in a driven state with driving frequency $\Omega = 0.125$ (blue).*

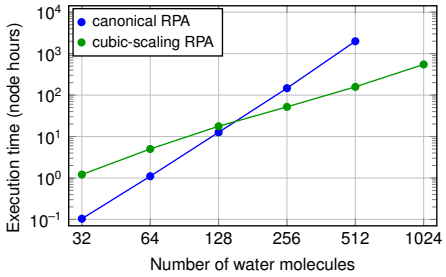

Figure 17: *Comparison of scaling between original and new $\mathcal{O}(N^3)$ RPA algorithm.*

crossover between field induced quantum tunneling and multi-photon absorption in electric-field driven Mott insulators. The weak-coupling and strong-coupling based Floquet+DMFT schemes will be used to investigate the properties of electron-phonon systems and multi-orbital Hubbard models which are excited by periodic electric fields or other periodic perturbations (modulations in the phonon potential, crystal fields, etc.).

3.3 Hutter and VandeVondele groups

Methods that include an explicit treatment of electron correlation can yield reliable results for a wide range of systems. They have the potential to provide both, high accuracy and general applicability. We are looking for algorithms to calculate the energy at these levels of theory while still providing an efficiency that allows applications to large systems and a sampling of many configurations.
New variations of ADMM [189] with charge constraints to speed up Hartree-Fock exchange have been implemented. These methods can also be used together with the post-Hartree-Fock methods (MP2, RPA, GW) [84, 86]. Analytic gradients and stress tensor are available for MP2. We investigated properties of liquid water using these methods and compared them with a series of density functionals [87, 88]. The G_0W_0 method has been implemented into CP2K [86] based on previous implementations of the correlation energy in RPA [190]. It displays high efficiency and good parallel scalability allowing for the study of large systems containing hundreds of atoms. Another project [85] is the development of a RPA correlation energy method with $\mathcal{O}(N^3)$ operations compared to the $\mathcal{O}(N^4)$ cost in the previous implementation (Fig. 17). The $\mathcal{O}(N^3)$-RPA method relies on the RI with a local metric, imaginary time and imaginary frequency grids and sparse matrix multiplications [191].
The VandeVondele group focused on simulations of electrochemical processes at the many-body electronic theory level with efficient algorithms for MP2 and RPA. For this, analytical spin-unrestricted MP2 forces [83] have been implemented. Applications to the hydrated electron by MP2 MD predicts a stable cavity structure (Fig. 18), and redox potentials of various aqueous species have been computed at the RPA level [89]. A multi-step integrator for path-integral MD (PIMD) enabling effective nuclear quantum effects with MP2 [99] has been developed, and nuclear quantum effects on the redox properties calculated by MD have been elucidated.

3.4 Marzari and Goedecker groups

a) *Spectroscopic properties from orbital-DFT* This project focus on the development and application of the Koopmans-compliant (KC) functionals [181][80]. The condition of Koopmans' compliance is naturally akin to that of enforcing a correct description of charged excitations, and thus leads to orbital energies that can be interpreted as the quasiparticle excitations measured in photoemission experiments [81]. Our most recent effort was toward (i) the development of an efficient scheme to capture orbital relaxation effects that naturally happens upon a photoemission process, and (ii) the validation of the method as a reliable tool for computing quasiparticle energies of extended systems and complex molecular systems. The implementations have been benchmarked on a comprehensive variety of molecular systems. The results for ionization potentials (IPs) improve when an orbital-dependent screening parameter is used and are typically comparable to those obtained with the best GW flavor. Theoretical photoemission spectra for the DNA and RNA nucleobases are in excellent agreement with experimental data [82]. We have also calculated the fundamental band gap of extended systems (Fig. 19).

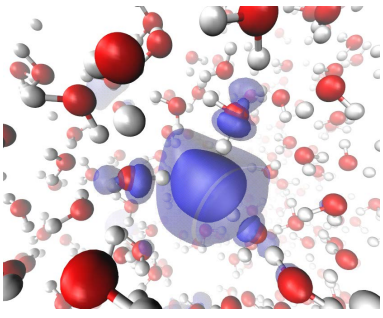

Figure 18: *Resolving longstanding controversies: the structure of the bulk solvated electron as obtained from MP2 based molecular dynamics, strongly supporting cavity formation.*

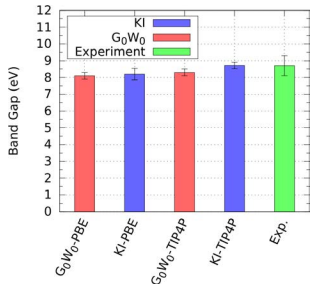

Figure 19: *Average band gap of liquid water from Koopmans-compliant functionals compared with G_0W_0 and experiments. The average is over two different NVT molecular dynamic trajectories at $\rho = 1\ g/cm^3$, generated with an* ab initio *DFT calculation (PBE) and a classical potential (TIP4P). The G_0W_0 results are adapted from [182].*

b) *Development of models, algorithms, and codes to include the effects of an aqueous environment in electronic-structure calculations* The computational study of chemical reactions in complex environments is critical for applications in many fields. The starting framework of the project is the self-consistent continuum solvation (SCCS) model [183]. It was extended to the calculation of optical spectra [90] and was coupled with periodic boundary correction schemes to handle aperiodic and partially periodic systems (Fig. 20) [91]. A novel solver for the generalized Poisson equation was developed and extended to the solution of the Poisson-Boltzmann problem, both in its linearized and in its fully non-linear formulation [92]. The resulting scheme allows the modeling of systems in the presence of an applied electrochemical potential, taking into full account the complex electrostatic screening coming from the solvent and the electrolytes. Efforts have been devoted to the fine tuning of the definition of the interface between the quantum-mechanical solute and surrounding environment, with the development of a soft-sphere model for the solute cavity [100]. Tuning of the model on experimental data of contact angle measurements allowed to improve its accuracy on surface properties of materials. The model and the optimized algorithms have been integrated into the BIGDFT and QUANTUM-ESPRESSO electronic-structure packages and are released as an independent library, suitable for integration in other codes, including packages developed outside MARVEL.

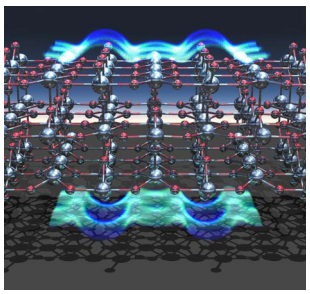

Figure 20: *Environment polarization surrounding a TiO_2 anatase slab.*

4 Contribution to overall goals

Simulation methods developed in HP3 are one of the core enablers for the vertical projects VP1 and VP2. They are also essential as base for the applications in HP4 and HP5. The developments of methods for strongly correlated systems is especially relevant for VP1. The new efficient implementation of MP2 and RPA methods are used in several projects in VP2. G_0W_0 and Koopmans functionals will be important for level alignment at interfaces, a crucial point in all electrocatalysis applications. Finally, the new developments for continuum solvent models has been adopted by several groups and will be key for the study of liquid-solid interfaces, as encountered in batteries, fuel cells, and electrocatalysis.

5 Collaborative and interdisciplinary components

The groups within HP3 are working mainly in bilateral collaborations. The Troyer and Werner groups have joined work on the sign problem in continuous-time QMC and on downfolding based on constrained RPA. The Hutter and VandeVondele groups have closely collaborated on the development and implementation of MP2 and RPA methods. They have also worked on algorithms for high-performance computing using the CP2K code. The work on continuum solvent models is a collaboration of the Marzari and Goedecker groups. Out of 48 MARVEL publications covering the work of HP3, 11 (23%) have been joined multi-PIs publications. Two algorithmic and method testing publications [99, 48] are collaborations with group leaders from other MARVEL projects. The methods developed in HP3 are made available to the MARVEL groups and to the scientific community in general through the simulation program packages and libraries (ALPS, TRIQS, QUANTUM-ESPRESSO, BIGDFT, CP2K). Applications of the methods within the other MARVEL projects are documented in the respective parts for this report.

Horizontal Project 4 HP4 — Advanced Sampling Methods

Project leader: Stefan Goedecker (UniBas)

Participating members: Stefan Goedecker (UniBas), Michele Parrinello (USI and ETHZ), Ursula Röthlisberger (EPFL), Berend Smit (EPFL)

Summary and highlights: New and improved methods were developed within HP4 to sample the potential energy landscape. First applications of these methods were done to help solving some of the key MARVEL challenges such as better materials for photovoltaics or for carbon capture. A common theme for all these efforts are quantities that allow to characterize materials. Depending on the context these quantities are called fingerprints, descriptors or collective variables. Work has started to compare the various fingerprints used by different groups and to assess whether they can also be used in other contexts. Methods that allow to study nucleation and growth will give guidance to synthesis efforts.

1 Main goals and achievements

Numerous problems in materials sciences require sampling the configurational space and to explore the potential energy surface. Various methods were developed within HP4 to perform such a sampling in an efficient way. The group of Goedecker has further optimized their minima hopping method and extended it from a method that can only find structures to a method that can also find in a fully automatic way reaction pathways. The group of Parrinello has introduced variationally enhanced sampling methods [101] to study the dynamics of systems on the free energy surface as well as to perform these simulations at constant chemical potential [102]. All these methods have already been applied to study perovskites that are under investigation in VP2 in the group of Röthlisberger as materials for photovoltaics. The minima hopping simulations of the Goedecker group found several hitherto unknown perovskite structures and the group of Parrinello started to study the nucleation and growth of these materials. This work builds on the highly successful studies of urea where the simulations of the Parinello group were able to show that different types of solvents lead to the growth of different structures [103, 104]. The group of Smit has developed descriptors for porous materials that allow to predict the performance of these materials for applications such as carbon dioxide or methane storage. The group of Röthlisberger has developed a method for optimizing the training datasets for machine learning [105].

2 Scientific outputs

The work in HP4 has lead to a large number of publications in high quality journals. The collaborations that have been established have lead to results that will soon be published in papers where several MARVEL group leaders are authors.

3 Progress of the different efforts

3.1 Investigations of perovskites (Ursula Röthlisberger — EPFL, Stefan Goedecker — UniBas, Michele Parrinello — USI and ETHZ, Berend Smit — EPFL)

a) *Structure predictions of perovskites* We started an extensive screening of the organic and anorganic perovskites that are of interest in VP2. We did these structure predictions both on the density functional level as well as using a home made force field. In this way we found both new crystalline structures as well as many defect structures that will be examined further to understand the dynamics of these materials. Fig. 21 shows two defect structures that are derived from the undesired delta phase of the methyl ammonium lead iodide crystal.

b) *Nucleation and growth of perovskites* Nucleation is a typical example of a rare event occurring on a timescale that is much longer than what atomistic simulations [103] can typically afford. Enhanced sampling molecular dynamics (MD) simulations [101] are therefore used to study the nucleation and surface growth of lead halide perovskites and the influence of different additives. More specifically, a full atomistic description of nucleation dynamics and thermodynamics will be explored, thus

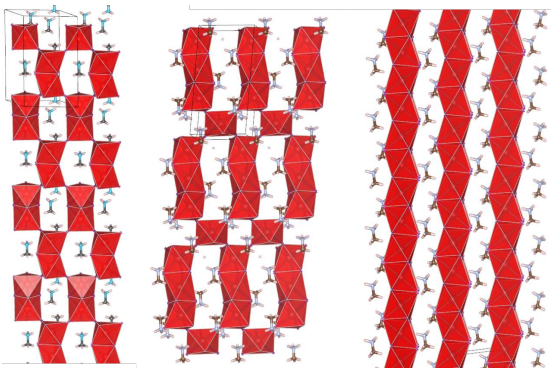

Figure 21: *Two defect structures (left and central panels) derived from the delta phase (right panel). Columns of octahedra (shown in red) which are of infinite length in the delta phase are broken up into shorter columns which are laterally displaced from each other along horizontal planes.*

paving the way towards a rational control of crystals grown from solutions. Until now we have focused on the development of accurate solute-solvent force fields parameters and standard MD simulations of fastest growing surfaces of methyl-ammonium lead iodide (MAPI) ($CH_3NH_3PbI_3$) in order to understand the adsorption and desorption mechanism of ions on the surfaces as described in the following section. In particular, we will compute free-energy profiles associated with the events of nucleation, adsorption and desorption of ions on different surfaces as well as in presence of additives. Such simulations will allow a deep insight into the complex nucleation process and crystal growth phenomena, thus enable a better control of the preparation process of perovskite solar cells.

The calculations of equilibrium crystal growth is mostly dominated by kinetics which control the morphology [102]. As a first step we are examining the MAPI surface growth dynamics and kinetics of fast (such as $\{100\}$) and slow growing (such as $\{001\}$) faces from solutions of different compositions of precursors (MAI and PbI_2) in GBL as solvent. We have observed the spontaneous adsorption of methyl-ammonium ions onto the $\{100\}$ surface in case of high concentrations only. However to understand the crystal growth kinetics, it is necessary to form a uniform perovskite arrangement of methyl-ammonium ($CH_3NH_3^+$), lead (Pb^{+2}) and iodide (I^-) on the top of the crystal seed as shown in Fig. 22. Simultaneously, we are focusing on improving the force field parameters of solute-solvent interactions. MD simulations of nucleation and crystal growth requires a reliable set of force field parameters of solute (($CH_3NH_3^+$), Pb^{+2} and I^-) solvent interactions. We are only interested in interactions of these ions with the most commonly used solvents such as dimethylformamide (DMF), gamma-butyrolactone (GBL) and dimethylsulfoxide (DMSO). Hence, with regard to lack of experimental data such as solvation free energies, static and dynamic electronic structure calculations are utilized to design force field parameters based on first principles calculations.

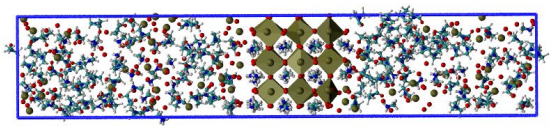

Figure 22: *A typical simulation cell for crystal growth of MAPI cubic phase in gamma-butyrolactone (GBL) as solvent.*

c) *Pore shapes of nano-porous materials* Modifying the pore structure of nano-porous materials can alter the performance in applications like carbon capture or methane storage by orders of magnitude [192, 193]. We assigned persistent diagrams to pore surfaces as seen by CH_4 and CO_2 to classify zeolites by their pore shapes, and screening for optimal ones as well as searching for similar materials in between different groups, e.g., finding the zeolites or hypothetical metal organic frameworks (MOF) most similar to an experimentally obtained structure of interest.
We were able to identify similar structures overlooked so far and to show that the pore-shape is relevant for the performance. Geometrically classifying top-performing zeolites for methane storage, we found that different shape-classes of zeolites have different heats of adsorption contrary to the established believe of an overall optimal heat of adsorption (Fig. 23) [194]. This shows new routes of optimization.

d) *Ionic conductivity of super ionic conductors* We are developing descriptors for ionic conductivity from the shape of potentials. This is relevant for the studies of super ionic conductors in VP2 performed in the group of Marzari. A first attempt to extract activation energy of conductivity from persistent diagrams ranked materials qualitatively correct. This gives a computationally cheap possibility to restrict to materials of interest. Furthermore, it is straight forward to detect minimal energy barriers for the different dimensionality of diffusion from persistent homological analyses. We are currently comparing different potentials and are in an exploration phase of identifying and in-

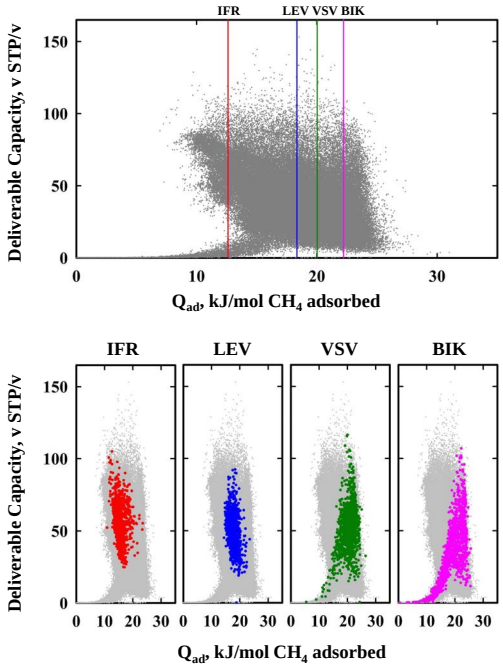

Figure 23: *Top: heat of adsorption and deliverable capacity of all zeolites. Bottom figures: highlighting the set of the 500 most similar structures to a references material (IFR, LEV, VSV, and BIK), showing that there are different optimal heats of adsorption for geometrically different classes.*

cluding more specific geometric properties determining diffusion, like the direction of the principal diffusion.

3.2 Minima hopping (Stefan Goedecker — UniBas)

A central tool for the exploration of the potential energy surface is the minima hopping method [162, 195]. This method allows to find in an efficient and entirely unbiased way low energy minima on the potential energy surface including the global minimum, i.e the ground state as well as low energy metastable structures. The moves in the minima hopping method are performed with molecular dynamics trajectories, whose energy is chosen such that the system preferentially escapes over low energy barriers from the catchment basin of the current minimum, exploiting the Bell-Evans-Polyani principle [196]. The exact local minima are then found by standard local geometry optimizations. The fact, that physically realizable moves are used, suggests to extend the method to a method that can find complex reaction pathways. This was done with the minima hopping global path search (MHGPS) method [106]. In the first publication we demonstrated for benchmark systems that it can find lower energy reaction pathways within less time than previous methods. Work has started to apply this method to real systems described on the density functional level and we expect that this method can solve challenging problems in materials sciences, such as transformations from one structure to another one.

Highly useful information about the potential energy surface is contained in so-called disconnectivity graphs, since they contain not only information about the energy of the local minima, but also information about the energies of the saddle points connecting these minima. Finding saddle points is numerically more expensive than finding minima and also the reliability of previously used method was not high enough to find, without human intervention, several thousand saddle points, necessary to set up a disconnectivity graph. For this reason we have developed a new saddle point search algorithm [107] which has a virtually vanishing failure rate and is nevertheless highly efficient. Alternatively we have also developed a method that allows to set up approximate disconnectivity graphs without calculating the saddle points [108]. The method depends on an empirical relation between the barrier height and the configurational distance of the two minima that are connected by the barrier.

3.3 Fingerprints (Stefan Goedecker — UniBas)

Configurational distances play an important role in many contexts. They are for instance required to determine in large crystal structure databanks which structures are similar or which structures are even identical, so that the duplicate structure can be eliminated. We have introduced a fingerprint for crystalline structures that fulfills all the properties of a metric and which is in particular independent of the choice of the crystalline unit cell [109].

3.4 Persistent homology (Stefan Goedecker — UniBas)

To avoid costly simulations of the behavior of each material in huge (hypothetical) databases, we developed computationally cheaper descriptors that ideally correlate with the property of interest or that restrict the number of materials for direct investigation. Organizing the database with respect to a new descriptor can lead towards new optimizing strategies.

We are focusing on describing, comparing and deriving information from geometric objects by adopting methods from a relatively new

mathematical theory called persistent homology [197]. Geometric information is most obviously contained in atom positions but also in shapes of potentials or of configuration spaces.

3.5 Variationally enhanced sampling (Michele Parrinello — USI and ETHZ)

The aim is to develop advanced phase space sampling methods for atomistic simulations of materials. In particular the goal is to develop variationally enhanced sampling (VES) [101], which is a new generally applicable collective variable based enhanced sampling method. What makes VES rather unique and novel is the fact that it is based on a variational principle [101], which brings considerable flexibility to the method, for example in the biasing potentials that can be employed and in the sampling that can be achieved.
So far the focus has been mainly on method development as described below. Going forward, the focus will increasingly turn to applying VES in atomistic simulations of materials within MARVEL.
We have improved the convergence behavior of VES by implementing an iterative scheme for achieving well-tempered sampling [110]. We have also implemented new basis set types (i.e. splines or Legendre polynomials).
We have shown that by employing approximate bias potentials we can efficiently explore high dimensional free energy landscapes [111].
We have extended VES such that it can be used to obtain kinetic information from atomistic simulations in an accurate and efficient way [112]. This approach has, for example, been applied to investigate the dissociation of molecular nitrogen on an iron surface.
We have shown how VES can be used to obtain free energy differences by employing a bespoke bias potential that is constructed from a model of local free energy surfaces, which only requires locally valid collective variables [113] (Fig. 24).
We have introduced a bias potential based on the model from classical nucleation theory that can be employed to accelerate nucleation events [114].
We have shown how VES can be used to investigate second-order phase transitions by directly parameterizing the phenomenological Ginzburg-Landau model [115]. In future work this approach will be applied to perovskites and other relevant materials.
We have been developing a general and modular software framework for VES that allows us to quickly implement and test new

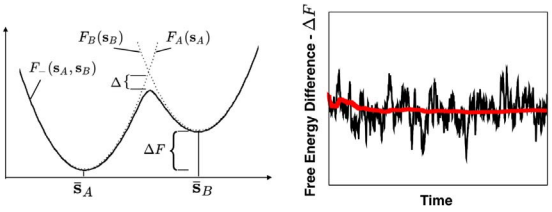

Figure 24: *Bespoke bias potential for obtaining free energy differences within VES.*

ideas. This framework is developed within the PLUMED 2 [198] enhanced sampling plugin that can be used with a wide range of molecular dynamics codes (i.e. CP2K, Quantum-ESPRESSO, LAMMPS, etc.). This framework will be made publicly available in the beginning of 2017 which will allow the wider scientific community to use VES and contribute to the development of the method.

3.6 Methods to study nucleation and growth (Michele Parrinello — USI and ETHZ)

The aim of this project is to develop enhanced sampling tools for the simulation of material's crystallization and crystal growth, overcoming the limitations of standard methods. The methods have been applied to predict the effect of solvent on the crystallization of urea taking into account finite size effects [103, 104]. We have also tested some of our methods to calculate nucleation rates reaching unprecedented time scales [116]. Since the chemical potential plays a crucial role in nucleation processes we have paid much attention to the calculation of the chemical potential and its control in solution [102, 117]. We have also developed a variational approach based on the use of the classical theory of nucleation that enhances the sampling of nucleation events [114].
Currently we have two important projects that we plan to develop during the next year,

a) *Collective variables for crystallization* Crystallization results from a trade off between entropy and enthalpy. Guided by this physical picture we have developed two collective variables that correlate with these quantities. These two variables do not require prior knowledge of the system and could be used for screening several compounds. We expect these variables to be useful in predicting structures stabilized by entropy like the superionic conductors and to illuminate the nucleation process. In Fig. 25 we show the usefulness of these variables in the study of Na crystallization.

b) *Chemical potential gradient* We have generalized the constant chemical potential

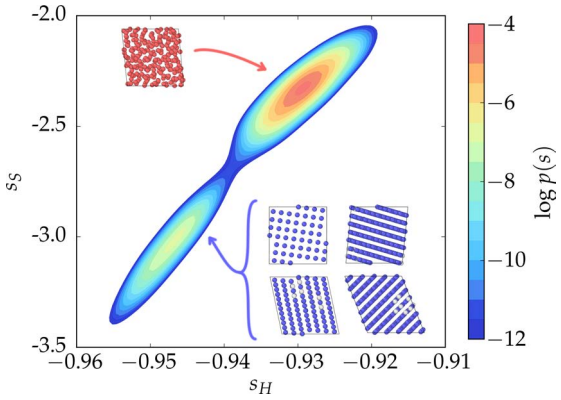

Figure 25: *Probability as a function of the collective variables connected to the enthalpy s_H and to the entropy s_S for Na at 350 K. A liquid and a solid BCC basin are observed and some characteristic configurations in each basin are depicted.*

method [102] to the case of constant chemical potential gradient. We have applied the resulting method to study the permeability of a zeolitic imidazolate framework-8 (ZIF-8) membrane to methane, ethane and ethylene [118]. This technique makes the calculation of this property straightforward and, hopefully, it allows to design novel materials with targeted permeabilities.

3.7 Optimization methods for fitting databases in machine learning (Ursula Röthlisberger — EPFL)

We have created a flexible, modular, and application-driven package of evolutionary algorithms (EAs), which we call EVOLVE. This package allows us to efficiently search chemical space, facilitating accelerated material and chemical design.

a) *Genetic optimization of training sets for improved molecular machine learning models* We have applied EVOLVE to the optimization of machine learning models of molecular properties. We have found using genetic algorithms (GAs) to optimize training set composition yields significant improvements to out-of-sample mean absolute errors (MAEs). Consequently, much fewer training examples are required to reach a certain level of accuracy. There are systematic trends in training set composition upon going from randomly generated to GA-optimized training sets. We have subsequently investigated the *a priori* selection of training data, however we have found this to be a non-trivial event with the insights gained upon the optimized training sets. Instead, we have found that using GA provides the means to generate training sets with better-than-random performance within databases for which no GA has been performed. This work is in submission [105].

b) *Compositional optimization of binary lead halide perovskites* Lead halide perovskites of the form ABX_3 (A = mono or divalent cation, B = divalent cation, X = halide anion) have recently become an intensely investigated area of research as light-harvesting materials due to low production costs and favorable band gap and charge carrier transport properties [199, 200]. The set of possible elements which can feasibly create perovskite materials is large, thus the search for the composition with optimal properties is a daunting task. During the third year of MARVEL, we have developed a computational protocol to perovskite design, through the coupling of EVOLVE, the QUANTUM-ESPRESSO *ab initio* code and AiiDA [59]. We are able to perform multi-objective optimization of perovskite composition with respect to a set of fitness functions calculated with *ab initio* accuracy. Here, EVOLVE provides trial compositions/configurations (Fig. 26), for which computation is managed by AiiDA. As a first test case study, this approach has been applied to lead halide perovskites with binary mixtures of monovalent cations (Cs^+, $(NH_2)_2CH^+$) with the aim of improving crystal phase stability, while maintaining optimal electronic properties for charge carrier transport and light absorption.

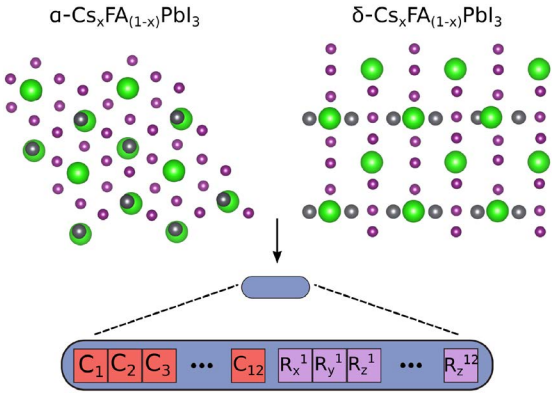

Figure 26: *Compositional encoding used within the optimization procedure for two separate phases. Trial compositional or configurational modification may only occur at the green spheres, which are typically samples from a finite temperature trajectory. These are represented by $C_{i...N}$ integers, corresponding to a library of molecular or atomic fragments. The remaining N x 3 positions correspond to the R_x, R_y and R_z rotation matrices of each fragment, allowing the procedure to additionally explore sterically hindered configurations.*

3.8 Structure predictions for other energy related materials (Stefan Goedecker — UniBas)

We further pursued our structure predictions for hydrogen rich materials that might be good superconductors and studied phosphorus-hydride compounds under high pressure [119]. We examined low density structures of silicon and found, in addition to the well known clathrate structures, a very large number of other structures with voids [120]. Some of these structures have a quite high absorption coefficient at the peak of the solar spectrum and would therefore be much better suited as a photovoltaic material than the standard diamond allotrope. Since synthesis efforts for several clathrate type silicon structures were already successful, there is hope that some of these predicted structures can be synthesized. We also studied the building blocks of metal atom doped carbon fullerenes, which are promising materials for superconductivity, thermo-electricity and notably hydrogen storage. By extensive minima hopping runs we first found the ground states for varying numbers of different metal atoms. This showed that previously assumed configurations were actually in many cases not the correct ground state. In the next step, we studied the behavior of the electron localization function for a single metal atom adsorbed on the fullerene for different types of metal atoms and could find rules that allow to predict the distribution of a larger number of metal atoms adsorbed on the fullerene (Fig. 27) without doing expensive structure prediction simulations.

3.9 Verification of electronic structure methods (Stefan Goedecker — UniBas, Nicola Marzari — EPFL)

Atomization energies of a test set of molecules were calculated with an unprecedented micro-Hartree accuracy. This became possible by using a multi-wavelet basis set that offers a high degree of adaptivity necessary for such all-electron calculations. These benchmark results allow us to assess the accuracy of other basis sets as well as of pseudopotentials and PAW schemes [121].

4 Contribution to overall goals and initial proposal

The initial MARVEL proposal stipulated that efficient sampling methods should be developed in HP4 that could help to solve problems in the vertical projects. This initial program outlay was followed. As described above, various methods were developed that are already applied to promote progress in materials discovery.

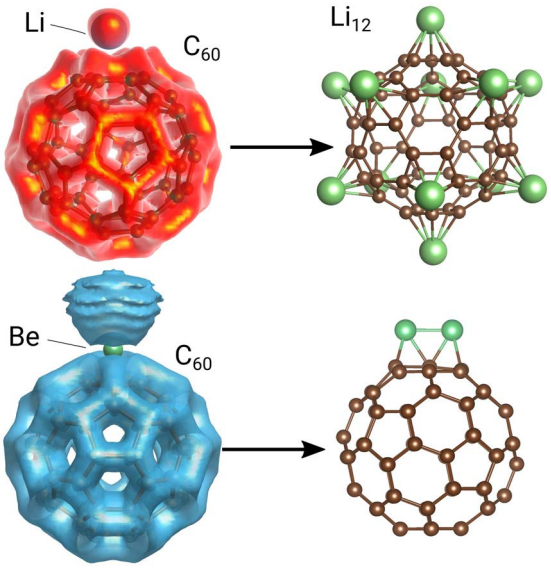

Figure 27: *By analyzing the electron localization function (ELF) for a single "probe" atom on the surface of a C60 fullerene we are able to predict if the metal atoms will form a cluster (bottom) or be homogeneously distributed (top).*

5 Collaborative and interdisciplinary components

The work within HP4 is organized around several central topics. At present several groups work already together on most of these central topics and the intensity of collaborations will even further increase. Concerning fingerprints, the groups of Ceriotti, Goedecker and Smit are involved. The methodological efforts of the groups of Goedecker, Parrinello and von Lilienfeld are supporting the investigations of perovskites in the Röthlisberger group. The groups of Smit and Marzari are developing descriptors for Lithium ion conductors. The groups of von Lilienfeld and Röthlisberger are working together on optimizing machine learning schemes. In a collaboration between the Goedecker and Marzari groups, a library to simulate complex wet environments was developed. The code can find the solution both for the Poisson equation with a spatially varying dielectric constant and for the Poisson-Boltzmann equation [92]. The first three year of MARVEL served as an initialization phase for collaborations and it is to be expected that these collaborations will lead to significant synergetic effects that will help to solve challenging problems in the coming years.

Horizontal Project 5 HP5 — Materials Informatics

Project leader: Alessandro Curioni (IBM)

Participating members: Alessandro Curioni (IBM), Michele Ceriotti (EPFL), Volkan Cevher (EPFL), Anatole von Lilienfeld (UniBas), Nicola Spaldin (ETHZ)

Summary and highlights: The goal of HP5 is to develop data driven methodologies for the acceleration of material discovery. The scientific community has been generating enormous amounts of valuable knowledge that has mostly remained confined into papers. Recently, it became evident that the data driven approach can unlock the huge potential of this data and allow for drastic acceleration of discovery. Indeed, HP5 researchers demonstrated that machine learning models can provide very accurate predictions of materials properties at a fraction of the cost and time needed by traditional approaches. Extracting the scientific literature treasure and structuring into searchable forms allows researchers to very fast learn from the collective experience of the community and thus move forward much faster. This is of course only the beginning. We have merely scratched the surface and already gotten strong evidence of the full potential of the approach.

1 Main goals and achievements

The goal of HP5 is to develop data driven methodologies for the acceleration of material discovery. To this end, we pursued significant advances in machine learning, knowledge representation and data driven modeling and simulation. In particular, the project developed methodologies for the prediction of materials properties, advanced technologies for data extraction from unstructured sources (e.g. papers) and the representation of knowledge as well as advances in optimization methods used to train machine learning based models. Moreover, our mission has been to link these advances with impact on the other vertical projects. We thus embarked into a number of well selected collaborations which are ongoing.

2 Scientific outputs

Ceriotti's group developed in 2016 new approaches to recognize recurring patterns at a molecular level [122], and to represent the similarity between materials and molecules [123], which can be applied for machine learning and for database science [124]. All of these developments have been made available as open source code through a GitHub repository (epfl-cosmo.github.io). These results have been presented by the group leader, as well as by Dr. De and Mr. Gasparotto, at about 10 seminars and conferences. Dr. De has won two poster prizes related to this line of research. In 2016, Anatole von Lilienfeld was appointed associate professor at the Free University of Brussels, BE, where he was awarded an "Odysseus" grant which he declined to return to Basel. MARVEL activities played a major role in his decision to come back. Also in 2016, Anatole von Lilienfeld was awarded an unrestricted research grant (US$ 100k) from Google, and a NRP 75 SNF "Big Data" grant as a co-PI in collaboration with Prof. Harbrecht (UniBas) on "Big data for computational chemistry: Unified machine learning and sparse grid combination technique for quantum based molecular design". Volkan Cevher received the IEEE Signal Processing Society best paper award 2017 (announced in December 2016) and in 2016 he received an ERC consolidator grant. Nicola Spaldin was awarded the L'Oréal-UNESCO Women in Science Prize in 2017. IBM team received the best paper award at IPDPS 2016 for linear cost stochastic matrix function approximation algorithms.

3 Progress of the different efforts

In the following, the various projects are described in detail. For each project, a summary of the first 33 months of MARVEL is provided. In addition to identifying the constituted research teams, particular emphasis is devoted to highlighting the specific goals, the achieved progress, and the future directions.

3.1 Predicting and rationalizing materials properties with machine learning (Michele Ceriotti — EPFL, Anatole von Lilienfeld — UniBas)

This project focuses on the development and application of advanced sampling and analysis techniques, inspired by machine learning. These methods are aimed at rationalizing structure/property relations, predicting the materials' properties while circumventing electronic-structure calculations, and navigating more efficiently large databases of compounds.

Building on our expertise on simplified representations of complex atomistic simulations (e.g. sketch-map (Fig. 28) [201, 202, 203]), we initially focused on pattern-recognition algorithms to identify elementary molecular motifs such as the hydrogen bond [122, 125]. To apply these methods to arbitrary materials it is crucial to obtain an effective representation of atomic environments and structures. To this aim, we leveraged the smooth overlap of atomic positions (SOAP) kernels [204], extended them to treat multiple elements and developed a strategy based on optimal-transport theory (REMatch) to combine them into a measure of similarity between molecules or solid structures [123]. With this approach one can represent the relationships between different conformers and phases of the same material, or give a bird's eye view of heterogenerous materials and molecular datasets. It also shows great promise for machine learning of materials' properties, and it allowed us to achieve predictions of molecular energetics with an error below 1 kcal/mol [123] for a benchmark set of compounds [205]. All of these algorithms have been made available as open-source software (GitHub repositories epfl-cosmo.github.io), and have been partially interfaced with the PLUMED code [198] so that they can be used to fuel accelerated-sampling methods. Work is underway to achieve further integration with AiiDA, and a web interface to analyze groups of structures using sketch-map will soon be included on the Materials Cloud. A proof-of-concept is available on sketchmap.org/pages/viewer/ISV/Silicon.

Besides these developments we have contributed to the use of advanced sampling methods within MARVEL, such as replica exchange (collaboration with Clémence Corminboeuf [126]), and accelerated path integral techniques (collaboration with Joost Vandevondele in HP3 [99]). In preparation for upcoming high-throughput studies, we have performed an in-depth analysis of the many free-energetic terms that determine the stability of different polymorphs of molecular crystals (e.g. paracetamol [127]).

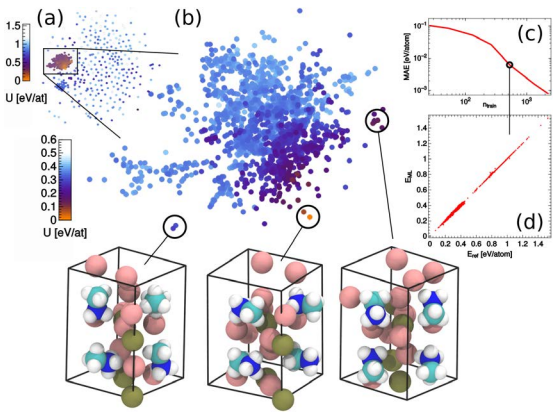

Figure 28: *(a) A sketch-map representation, based on bespoke crystal-structure fingerprints, of the MAPbI polymorphs found by minima hopping shows a large spread in energies, and a variety of lattice symmetries. (b) Many stable structures are clustered together, and they are found to all have a perovskite structure, and differ by defects and the orientation of methylamine units. (c) Using SOAP-based descriptors, one can also predict the cohesive energy of all the structures, with a mean absolute error below 5 meV/atom when using 500 structures for training, as shown in the (d) correlation plot.*

3.2 Advanced technical document understanding for the discovery of novel materials (Alessandro Curioni — IBM, Nicola Spaldin — ETHZ)

In this project, we are focused on the big data aspect of novel materials engineering. It is widely accepted that a treasure trove of information with regard to materials exists in the published literature. However, this data is not accessible by machines, typically due to the presentation of the data (natural language, complicated tables, etc.) as well as due to unstructured document formats (such as pdf). To tackle this problem of data-extraction and data-querying from unstructured data sources, we have developed three key technologies over the last three years.

1. An automatic pdf-parsing and annotation tool, allowing us to obtain a semantic representation of the original pdf-document in JSON format [128, 129].

2. NLP annotators for text, which allow us to detect material formulas and their properties in the semantically parsed documents from item 1.

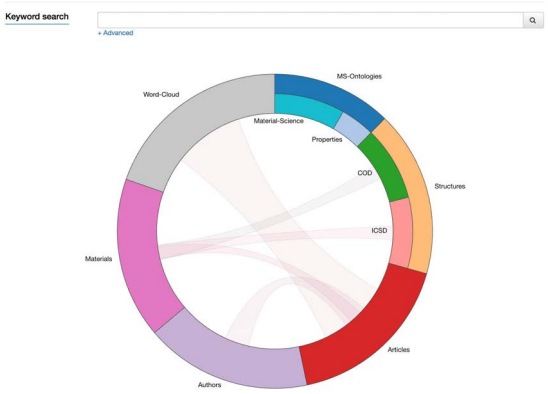

Figure 29: *Screenshot of the user interface for the knowledge graph for materials.*

3. A platform for the creation and querying of large knowledge graphs (KG). The latter allows us to ingest the parsed and annotated journal articles from item 2 and query the data encapsulated in them in an intuitive way.

It is important to realize that the consecutive application of these three technologies forms a pipeline to extract and query data from journal articles in pdf format. Such a pipeline allows us to answer questions such as *"list me all materials that are known BCS-superconductors"* via a simple user interface, shown in Fig. 29. Due to the wide scope of each section item, we dedicated a year of work on each. In the first year, we developed a scalable platform for the creation and querying of KG. This required us to investigate how to translate material science related questions into algorithmic workflows on the graph. We discovered that a straightforward application of these algorithms on advanced queries are computational expensive. Therefore, we came up with a novel algorithm, which was published at IPDPS and awarded with the best paper award [130]. In the second year, we focused primarily on the data gathering, cleaning and ingestion into the knowledge graph. Part of this work entailed the ingestion of crystallographic databases (ICSD and COD) as well as various digital literature resources (ArXiv, Pubmed, USPTO and Wikipedia). Most of the work went into the development of NLP annotators to detect chemical formulas and material properties with their numeric values. This allowed us to create edges between the material-nodes and property nodes of the KG. In the third year, we focused on the ingestion of literature resources in pdf format. In order to obtain very high accuracy, we build a pdf-parsing pipeline, where the user can train a machine learning (ML) algorithm via manual annotation in order to determine the semantic role of each text-cell. After the annotation of around 30 pages, the ML typically obtains around 99% accuracy and we can then use the semantic labels of each textcell to reconstruct a semantic representation of the pdf-paper in JSON format. This latest work has led to two papers [128, 129], currently in submission. In the next year, we plan on opening up the KG to selected users and start verifying the predicted material properties with simulations done through the AiiDA platform.

Beyond the application to solid state electrolytes (VP2) we started an additional one aimed at incorporating magnetic symmetries into open-source crystallographic databases, in collaboration with Nicola Spaldin (ETHZ) and Thomas Schulthess (CSCS and ETHZ). In fact, current crystallographic databases, such as ICSD or the Materials Project [206], contain information about crystal chemistry and structure of a broad range of materials and are increasingly used in searching for materials with specific properties and functionalities as a starting point for new materials design. No existing database, however, contains detailed information about magnetic properties. The goal of this project is to build up databases that include comprehensive information on magnetic symmetry, complementary to existing open-source crystallographic databases. This information will be invaluable in searching for materials with functionalities such as magnetic response to an electric field, exotic superconductivity and tunable transitions between insulating and metallic behavior.

In this initial phase of the project we have begun to use IBM's cognitive computing approach to search existing literature and identify descriptions of magnetic properties in it, in order to extract them into a well-defined machine-readable format. IBM and CSCS will collaborate to install and support a system that allows access to an API supporting the extraction of knowledge entities from papers. The information will be extracted and inserted into a public database (IBM) that is accessible to outside users. Negotiations with publishers will be pursued to extend license agreements to allow for automated searching of literature (ETHZ Library).

In a second phase, key areas of information deficiency will be identified (IBM) and additional information will be generated using first-principles calculations (ETHZ Materials Theory and CSCS) and further incorporated into the database. The database capability will ultimately be used (ETHZ Materials Theory) in

the search for and design of novel magneto-electric materials.

3.3 Machine learning and perturbation theory in compositional space (Anatole von Lilienfeld — UniBas)

To accelerate computational materials design and discovery we develop rigorous new structure-property models using (i) machine learning or (ii) perturbation theory.

a) *Machine learning* Building on previously developed predictive machine learning (ML) models [207] of molecular properties [208], we have carried out multiple studies aiming to gain a deeper understanding of these methods, and to use it for the development of improved methods. Specifically, we introduced a ML based correction, called Δ-ML model, of lower-lying levels of quantum chemistry methods, such as PM7 and DFT. For many molecular quantum and thermochemical properties, we showed that computationally demanding and highly accurate quantum chemistry results can systematically be approached at the cost of the baseline method augmented by the ML correction [131]. We also showed that atomic properties, such as atomic multipole-moments, NMR shifts, or atomic forces, can be predicted by atomic ML models [132, 133]. Furthermore, ML models of electronic excitation energies have also been demonstrated to bridge the gap between time-dependent DFT and coupled-cluster accuracy [134]. ML models of properties of solids have also been developed [135]. We succeeded to contruct a ML model which reaches DFT accuracy for predicting formation energies of new crystals in the elpasolite form

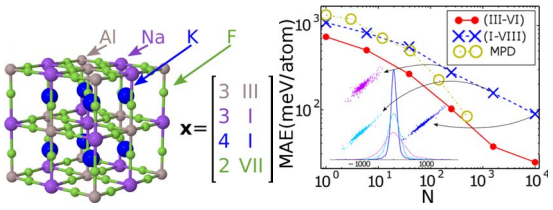

Figure 30: *Machine learning (ML) models of formation energy of crystals reach DFT accuracy. Left: any crystal of elpasolite symmetry can be represented by a 4×2 matrix, specifying period and group for the constituting elements, e.g. $AlNaK_2F_6$. Right: out-of-sample mean absolute errors (MAE) for formation energies of crystals from small (red, main group elements III-VI) or large (blue, main group elements I-VIII) elpasolite dataset, and from materials project database (yellow, few elements). Inset scatter plots and error distributions indicate systematic improvement for large dataset ML models.*

(Fig. 30), and we have used it to discover ∼ 90 previously unknown elpasolites [136]. Most recently, we have shown that uniqueness and target similarity of a compound's representation play a crucial role in learning rate and off-set. We have used this insight for the generation of ML models with unprecedented predictive power and efficiency [137].

b) *Perturbation theory* In accordance with the original proposal, we investigated the performance and limitations of first order perturbation theory for predicting the response of properties due to changes in chemical composition. Building on preceding results [209], we have studied an array of properties and systems including relative energies and structures in ionic crystals, metals, or molecules. Consistent and comprehensive numerical evidence suggests that first order based estimates of relative energies can reach strong predictive power, even chemical accuracy, if the compositional changes occur for fixed "vertical" compositional changes and among heavy elements in the periodic table [138, 139, 140].

3.4 Submodular subset selection for materials prediction (Volkan Cevher — EPFL)

Machine learning promises unprecedented opportunities for computational materials science, such as prediction of materials properties for rapid prototyping and proposing new material configuration with desired properties. In this setting, we have focused on the neural networks as well as the kernel ridge regression machineries and developed methods for making them more accurate, flexible, and scalable. Since we joined the project last year, along with Christoph Koch at EPFL, we have tasked two project students with implementing new techniques for training neural networks for materials discovery. The new method improves the speed and quality of the learning results and the result [141] was published at the premiere machine learning conference NIPS. Several groups inside MARVEL are interested in such as result, including Alessandro Curioni's, Anatole von Lilienfeld's, Michele Ceriotti's, and Christoph Koch's.

In quantum chemistry, computing certain properties, such as atomization energy of molecules, is computationally challenging [210]. For instance, while the kernel methods (such as kernel ridge regression, Gaussian processes, etc.) currently obtain the state-of-the-art prediction results, their computation scales as $\mathcal{O}(n^3)$, where n is the dataset size. Moreover, storing the kernel

matrix K and solving the associated linear system is prohibitive when n is large. One way to overcome these issues is to select a small subset of data while maintaining an information diversity.

A popular criteria for active set selection is the informative vector machine (IVM) [211], where we select a set S that maximizes the mutual information utility $f(S) = \frac{1}{2}\log\det(I + \sigma^{-2}K_{S,S})$. Here $K_{S,S}$ is the submatrix of K, corresponding to rows/columns indexed by S, and $\sigma > 0$ is a regularization parameter. This utility function is monotone submodular, as shown in [212].

To this end, we are interested in finding the smallest subset that achieves a chosen utility level, which is a submodular cover (SC) problem. Despite the fact that the standard SC problem is extensively studied, all the proposed algorithms heavily rely on having access to the whole ground set during their execution.

However, for large scale materials databases, this assumption does not hold. For instance, when the dataset is being generated on the fly or is too large to fit in memory, having access to the whole ground set may not be feasible.

Similarly, we may have some restrictions on how we can access the data. Namely, random access to the data can simply be not possible, or we might be restricted to only accessing a small fraction of it. In all such scenarios, the optimization needs to be done on the fly.

Hence, we initiate the study of the classical submodular cover (SC) problem in the data streaming model which we refer to as the streaming submodular cover (SSC). Our result is specifically demonstrated for materials subset selection tasks for kernel ridge regression and is accepted to the premiere machine learning venue NIPS 2016 [142].

We apply the new method to the IVM objective where we use the Gaussian kernel $K_{ij} = \exp(-\frac{\|x_i - x_j\|_2^2}{2h^2})$, and we set the hyperparameters as in [210]: $\sigma = 1, h = 724$. The dataset consists of 7k small organic molecules, each represented by a 276 dimensional vector. We set $M = 2^{15}$ and vary Q from $\frac{f(V)}{2}$ to $\frac{3f(V)}{4}$, and α from 1.1 to 2.

The reason why we selected such a small dataset is the following: for this dataset, we have access to an expert selection (namely, Matthias Rupp), which creates the baseline. Our algorithm achieves the same level of performance with respect to this baseline; However, it is fully automated. In the future, we would like to pursue this approach on bigger datasets.

4 Contribution to overall goals and initial proposal

HP5 remained firmly focused on the overall goal to accelerate material discovery. In particular, we are following a data driven approach that utilizes existing data (coming from models, simulations and publications) to design machine learning methods that can predict properties of materials and find interesting new material candidates. To this end, we developed a systematic methodology to extract data from the scientific literature and organize it in a searchable way.

5 Collaborative and interdisciplinary components

We have embarked in cross collaborative research projects with VP2 (Marzari) for the integration of the AiiDA platform and VP1 (Spaldin) to expand the knowledge graph to other fields of interests such as multiferroic systems with the help of CSCS (Schulthess) and ETHZ library. We are in the process of providing our S/W and methods as a service to the MARVEL community, initially, and to the general community subsequently. Moreover, collaborations are ongoing within and outside MARVEL to apply these approaches to different molecular and materials' problems. These include a set of more than 50'000 stable conformers of oligopeptides ([124], in collaboration with Carsten Baldauf from FHI-Berlin), and several hundreds low-energy polymorphs of materials for molecular electronics (in collaboration with Graeme Day, from Southampton). Within MARVEL, HP5 is currently collaborating with Clémence Corminboeuf (molecular switches), Stefan Goedecker (structural fingerprints analysis), Nicola Marzari (2D materials), Carlo Pignedoli (graphene nanoribbons) and Anatole von Lilienfeld (machine learning algorithms).

Platform Project 6 PP6 — Informatics

Project leader: Thomas Schulthess (CSCS and ETHZ)

Participating members: Thomas Schulthess (CSCS and ETHZ), Nicola Marzari (EPFL)

Summary and highlights: The Informatics platform is delivering, ahead of schedule, its objectives of (1) developing a materials' informatics infrastructure to manage high-throughput calculations, organize all data with full provenance and reproducibility, and encode in robust workflows the calculation of complex materials properties that also allow for continuous testing, verification and validation of the calculations; (2) developing a portal for the dissemination and sharing of the curated data, of the entire provenance and data tree, and also of educational materials and work tools for the community (additional objective with respect to the original proposal); and of (3) developing a shared software infrastructure, in the form of the SIRIUS domain-specific library, able to unlock the power of emerging supercomputing platforms based on multi-core, GPU, and accelerator architectures. These objectives are also supported by a close participation of CSCS staff in the provisioning of services and developing of shared solutions.

1 Main goals and achievements

1.1 AiiDA

AiiDA — aiida.net — is the open-source (MIT license) materials' informatics infrastructure that provides the MARVEL community and the scientific community at large with an "operating system" able to deal most efficiently with the complex requirements of computational science, including the automation of high-throughput simulations on remote resources; the storage, preservation, provenance, and efficient searching of data; the development of a working environment where workflows connecting different and complex codes are constructed; the sharing and dissemination of data. AiiDA fully implements the four pillars of the ADES model [59]. (1) **Automation** of job execution: input file creation, copy of files to remote supercomputers, job submission, file retrieval and parsing. (2) **Data**: calculations, their inputs and their results are stored in a database, in a format suitable for querying. (3) A high-level **Environment** for materials scientists to express their problems abstractly using workflows. (4) Import/export capabilities to facilitate **Sharing** of parts of the private AiiDA databases with collaborators, as well as uploading calculations to a public portal (and in particular to the Materials Cloud).

1.2 Materials Cloud

The second objective is to develop a comprehensive portal for computational materials science — materialscloud.org — that provides an online environment integrating the various resources needed by scientists to pursue their research objectives. These are grouped into four categories: (1) **Learn**: educational content with a broad coverage of materials science topics addressing learners of various backgrounds. (2) **Work**: a collection of interactive tools that embody the spirit of *software as a service* and provide the ability to carry out complex calculations and processing data without domain expertise (Fig. 31). (3) **Discover**: a repository of curated datasets of material properties, to disseminate results to the wider scientific community. (4) **Explore**: an interactive online AiiDA database contributed by NCCR groups, to enable seamless sharing and collaboration.

Another objective of Materials Cloud is to have a platform that realizes the FAIR principles [213] (Findable, Accessible, Interoperable, Reusable) for the Data Management of the MARVEL community.

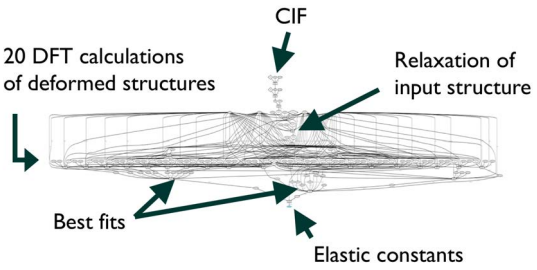

Figure 31: *An AiiDA graph representing a typical turn-key solution; in this case, the automatic calculation of the elastic tensor for an arbitrary crystal structure.*

1.3 SIRIUS domain specific library

The third objective is to develop the software solutions that allow to run and validate state-of-the-art DFT codes on flagship architectures, starting form the CSCS hybrid supercomputer Piz Daint (Cray XC50 nodes of Intel Xeon E5-2690 v3 @ 2.60GHz, 12 cores, 64GB RAM and NVIDIA Tesla P100 16GB GPUs). For this, the SIRIUS [143] domain-specific library for electronic-structure calculations is being developed with the goal to separate and optimize the low-level quantum engines from the electronic structure codes [144]. As discussed in more detail later, the library supports several diagonalization-based methods, includes a hybrid CPU-GPU implementation of a complete DFT loop and is fully compatible with Quantum-ESPRESSO (plane-wave, pseudopotential) and Exciting (all-electron).

1.4 CSCS service provisioning

CSCS is responsible for the hardware infrastructure of MARVEL as well as provisioning core services, such as computing, storage, database, identity management and security. Furthermore, CSCS and EPFL are now partners in the H2020 MaX centre of excellence on Materials Design at the eXascale, and are starting to work with other HPC centres (starting with CINECA and Jülich) to build a federated infrastructure.

2 Scientific outputs

AiiDA has been thoroughly described in [59], while the first pseudopotential verification and validation effort (published in *Science* [121]) has led to the curation of a *Standard Solid-State Pseudopotentials* (SSSP) library whose accuracy fully matches the 7 all-electron codes discussed in [121]. Notable has also been the outreach activity with 8 AiiDA tutorials both for users and developers, reaching close to 300 participants; many of the events have been co-sponsored by centres outside MARVEL.

3 Progress of the different efforts

3.1 AiiDA as a materials' informatics platform

There have been five code releases since the first open-source version 0.4.0 (Feb 2015). A paper describing the platform and the ADES model has been published [59]. We have also spent significant efforts to strengthen the user support via the extensive code documentation (aiida-core.readthedocs.io), a mailing list for general discussions and for support, and 8 tutorials. Currently, the AiiDA team is composed of 13 members, including two computer scientists, and the code has over 30 contributors (also including the various plugins). The main developments of the last three years include:

2014 – 2016 Job scheduler plugins (Torque, PbsPro, Slurm, LSF, SGE, and "direct" to emulate a scheduler).

2014 – 2016 Unit tests for the vast majority of the code, and continuous integration at every commit.

2014 – 2016 Automated and robust workflows to enable high-throughput calculations using Quantum-ESPRESSO and: detect if a structure is magnetic, metallic, …; scan crystal structures and identify 2D substructures; calculate phonon dispersions using both the QE ph.x code and PhonoPy; initialise and run molecular-dynamics simulations.

2014 – 2016 Many code plugins implemented, often triggered by the AiiDA tutorials, ensuring strong collaborations of the AiiDA team with other groups: Quantum-ESPRESSO (PW, CP, PH, PP, PROJWFC, DOS, PDOS, NEB), WANNIER90, Yambo, GPAW, ASE calculators, Phonopy, NWChem, CODTools, CP2K, FLEUR, Exciting, SIESTA, i-PI, VASP. Moreover, extension of many data classes to support automatic generation of the *k*-point path [145], to support MD trajectories, Gaussian and atomic-orbital basis sets, Wannier functions, interatomic force constants.

2015 Importers and exporters between AiiDA crystal structures and ASE (wiki.fysik.dtu.dk/ase/) and pymatgen (materialsproject.org). Importers from many structural databases: ICSD, OQMD, NNINC, PCOD, MPOD, TCOD. Exporter of results including the full calculation provenance to TCOD (crystallography.net/tcod [172]).

2015 A new optimised backup script scaling well to repositories with over tens of millions of nodes.

2015 – 2016 Abstracted AiiDA from the previous ORM (Django) and implemented a second one using SQLAlchemy+PostgreSQL 9.4 with JSONB fields, obtaining a 50x speed-up for important database queries.

2016 Advanced querying tool (QueryBuilder) supporting graph queries with a database-agnostic and user-friendly interface.

2015 – 2016 Support for workfunctions; re-designed workflow engine to ease the implementation of workflows, providing: automatic provenance tracking; trivial reuse of workflow steps and workflows themselves; debugging support and fast-forwarding.

2016 Multiple profiles/databases switchable at runtime.

2016 Improved plugin API to allow for multiple executables within the same scheduler job, so as to support codes that require pre- or post-processing (Yambo, FLEUR, WANNIER90, i-PI, ...).

2016 Improved plugin infrastructure, encouraging plugin development and automated testing in repositories independent of AiiDA.

2016 Tutorials released in a complete downloadable virtual machine.

2016 Deployment of AiiDA and related services via docker (and docker-compose).

Planned research for next year

(a) Improvements of the sharing protocol (synchronization of profiles, incremental sharing).

(b) Full support of AiiDA in combination with the Materials Cloud portal and integration with services at CSCS (database, object store).

(c) AiiDA version 1.0 (to be released in a few months) with focus on stability, optimization of performance, efficiency, and ergonomy.

Synergies with other computational and experimental efforts We are part and periodically coordinate with two H2020 projects: the e-infrastructures centre MaX ("Materials Design at the eXascale") and the integrating infrastructure NFFA ("Nanoscience Foundries & Fine Analysis"), both having AiiDA as a core component for the management of computer simulations. We are collaborating closely with COD (crystallography.net [172]). We interact with the Materials Project (materialsproject.org [206]) and OQMD (oqmd.org [214]) to maintain interoperability (converters and/or exporters are available into AiiDA). We are part of the Optimade working group (www.optimade.org), to deliver a common REST API to make different databases interoperable. We are in close interaction with Atsushi Togo (Kyoto Univ.), author of the SPGLIB and phonopy packages. Both are now already usable from AiiDA, and we work on common workflows for running phonons independently of the computational code used.

3.2 The Materials Cloud portal

The software architecture of the Materials Cloud portal reflects the decision to decouple server and client side. The server side relies largely on AiiDA for calculation and data storage, query and management. The communication between client and server is enabled by a REST API (that we developed using the *Flask* microframework) to make AiiDA resources available and querable via HTTP requests. Multiple authentication protocols are already implemented (including HTTP basic authentication and token-based). Since the start of the Materials Cloud subproject (about one year), considerable effort has been directed to the development of the front-end based on the AngularJS framework. Each of the four sections of MaterialsCloud are already populated with one or more working functionalities.

In particular, the **Explore** section provides a graphical interface to browse remotely the AiiDA database. It is possible to view the database either as a list of nodes, taking advantage of filtering, sorting, and pagination features, or as a graph that highlights the input/output relationship between nodes. Additional views provide details of selected nodes with interactive content visualization of its content: e.g. 3D atomic viewer for crystal structures, thanks to the embedding of several JavaScripts plugins (Kendo UI, Highcharts, ngTable, ChemDoodle) into the AngularJS framework. The **Discover** section is being enriched with a collection of curated sets of data contributed by different research groups. These include for example the sketch-map visualization of similarity of crystal structures, and curated databases of layered materials with their binding energy, of thermochemical properties of solids, of 2D and 3D covalent organic frameworks and of metal organic frameworks. Curated datasets are tightly coupled with the Explore section, so that their full provenance is easily obtainable and browsable. In the **Work** section we aim to provide users with tools to build new knowledge out of existing data. We

have already integrated SeeK-Path (materials-cloud.org/tools/seekpath) [145], an advanced *k*-point path visualizer that provides recommended band paths in a standard and automated way, following the prescriptions and conventions of crystallography, as well as the SSSP pseudopotential verification effort, giving users the flexibility to build custom plots to compare interactively pseudopotentials. The **Learn** section contains a collection of learning materials, including: the video lectures of the 2009 Santa Barbara Summer School on *ab initio* calculations; a selection of exercises and tutorials on Quantum-ESPRESSO; videos from the Jun 2016 3-day AiiDA tutorial; videos from the 2017 2-week ICTP Advanced Workshop on High-Performance & High-Throughput Simulations; and the MARVEL distinguished lectures. This section is powered by the slideshow (slideshot.epfl.ch) technology that combines video and slides with advanced synchronization features.

As explained below, four projects have been started in collaboration with CSCS (involving monthly online meetings) to ensure that Materials Cloud can run and scale on the federated services being developed and deployed at CSCS.

3.3 The SIRIUS domain-specific library

As a partner of the MARVEL Informatics platform, ETHZ (CSCS) is working on two software solutions to allow to run and validate DFT calculations on the flagship hybrid supercomputer Piz Daint: the SIRIUS library and the AiiDA plugins for Exciting FP-LAPW code. SIRIUS [143] is a domain-specific library for electronic structure calculations which is being developed at CSCS with the goal to separate and optimize the low-level quantum engines from the electronic structure codes [144]. The library supports several most popular diagonalization-based methods, such as plane-waves (PW) pseudopotential and projected augmented waves (PAW), as well as full-potential linearized augmented plane waves (LAPW). The SIRIUS library is available under the BSD license and includes a hybrid CPU-GPU implementation of a complete DFT ground state loop (Hamiltonian diagonalization, density construction, generation of effective potential, symmetrization and mixing), for PW and LAPW basis sets (Fig. 32).

The following features have been implemented in SIRIUS since the start of the MARVEL project: (a) scaling of LAPW engine to simulate large unit cells [146]; (b) iterative solver for

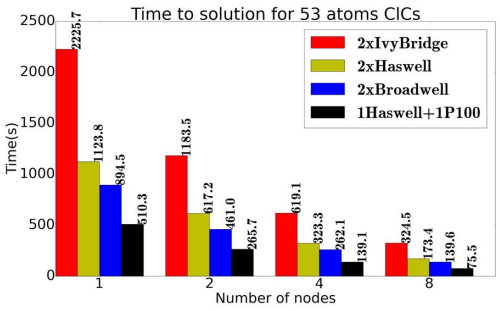

Figure 32: *Performance benchmark of the SIRIUS library running* Quantum-ESPRESSO *in a 144-atom unit cell of SiO_2. The runs we performed on dual-socket Ivy Bridge (16 cores), Haswell (24 cores), Broadwell (36 cores), and on a hybrid node with 12-core Haswell + NVIDIA Tesla P100 card.*

LAPW basis; (c) plane-wave pseudopotential (norm-conserving, ultrasoft, PAW) engine with collinear magnetism.

We plan to turn this library into a supported product, that we will extend as follows: (1) engage the community code developers or advanced users to work together on the library API, and interface SIRIUS with Quantum-ESPRESSO and Exciting; (2) implement atomic forces in PW pseudopotential and LAPW full-potential; (3) implement non-collinear magnetism and spin-orbit correction in PW pseudopotential; and (4) implement infinite-order regular approximation (IORA) in LAPW. Finally, for what concerns the AiiDA plugin for the Exciting code, the current version is already able to compute ground-state energy and evaluate the equation of states, and we are now supporting also the calculation of stresses, forces, atomic relaxations and variable cell relaxations. This AiiDA plugin is essential for the validation of results published on Materials Cloud against a full-potential LAPW code.

3.4 CSCS service provisioning

The necessary computing infrastructure was installed at CSCS at the end of 2014. Installed hardware includes 180 dual-socket compute nodes (2x Intel Haswell 12-Core, E5-2690 v3 @ 2.6 GHz), with 64 GBytes of memory (DDR4 @ 2133 MHz) and is clustered to the Cray XC40 supercomputer Piz Dora. MARVEL compute nodes have a full access to the scratch filesystem of 2.7 PetaBytes shared with Piz Daint. Both systems have been now integrated into one single upgraded XC50 machine. The available resources were distributed among the different MARVEL projects as a quota of node-hours per quarter. Production workload be-

gan on Apr 1st, 2015 and resources have been utilized steadily since. An initial amount of 100 TB of permanent storage was also distributed among all MARVEL projects, which was extended to 200 TB at the beginning of 2016. Quarterly reports are being regularly issued by CSCS with accounting records and other useful statistics.
Besides continuing operations and following up on the different aspects of the MARVEL-CSCS collaboration, a series of activities have started in Q4'2015 between members of AiiDA, Materials Cloud and CSCS to deploy proof-of-concept services to explore the possibilities of a federated infrastructure (between Jülich, CSCS and CINECA). The first project in Q4'2015 focused on the storage service (initially based on iRods) to help data dissemination. This established the base for further collaboration between members of AiiDA and CSCS teams to write requirements and use cases for MARVEL. This has led in Q4'2016 to the deployment of four proof-of-concept services where the Materials Cloud service can run: web servers, databases (Postgres), object storage (OpenStack Swift) and authentication and authorization infrastructure (AAI). The first three services are in testing phase and are expected to be functional by Apr 2017. Given this close collaboration between CSCS and EPFL, a meeting is scheduled monthly to discuss progress on the different areas and strengthen the collaboration.

4 Contribution to overall goals and initial proposal

We have realized very close and fruitful synergies between the software efforts (AiiDA) and the hardware (SIRIUS for performance, and the supercomputing center CSCS for service provisioning, integration of the front-end, back-end, database, and storage), that are not only essential to the deployment of the design and discovery projects of phase 2, but also represent one of the pioneering efforts worldwide. The AiiDA infrastructure is a fairly unique and very advanced effort in offering an "operating system" for simulations, and has repeatedly been praised (also by the Scientific Advisory Board). Other efforts like the UNICORE middleware; the Fireworks workflow management system and pymatgen from the Materials Project; the Atomic Simulation Environment ASE (DTU and Stanford) provide complementary functionalities that are compatible with AiiDA. The objectives of the Materials Cloud are unique in their offering of educational material or extensive data with full provenance. For the curated data, they are complementary to the US effort of the Materials Project and the OQMD — providing some needed verification, being performed with a code different from VASP. Last, the SIRIUS library also offers a unique opportunity to exploit new and complex architectures (e.g. GPUs, accelerators) with current electronic structure codes.

5 Collaborative and interdisciplinary components

Up to now we have hold 8 AiiDA tutorials both for users and developers, reaching 300 participants. An additional tutorial is already scheduled for May 2017 in Lausanne. Some of the tutorials have been co-sponsored by centres outside MARVEL, such as the MaX CoE, Psi-k, CECAM, ICTP. We constantly coordinate multiple efforts, including the various code plugin developments taking place in multiple groups; biweekly meetings with the full AiiDA team, including the team at Bosch RTC in the USA; the coordination with various computer centres (CSCS, CINECA, ...) toward the deployment of AiiDA directly on the supercomputers. In semester projects, a group of eight Computer Science students from Prof. Koch's "Big Data" course investigated possible extensions of AiiDA using other SQL and NoSQL databases, putting the grounds for the multi-backend support. In fall 2016 two students from the Indian Institute of Technology investigated possible database optimisations for AiiDA. A collaboration with a company has been initiated, involving scientific consulting and an AiiDA license for support and new developments not yet included in the public release.

Platform Project 7 PP7 — Experiments

Project leader: Frithjof Nolting (PSI)

Participating members: Frithjof Nolting (PSI), Michel Kenzelmann (PSI), Pierangelo Gröning (Empa), Raffaella Buonsanti (EPFL), Claudia Cancellieri (Empa), Thomas Lippert (PSI), Marisa Medarde (PSI), Daniele Pergolesi (PSI), Wendy Queen (EPFL), Marco Ranocchiari (PSI), Marta Rossell (Empa), Christian Rüegg (PSI), Thomas Schmidt (PSI), Thorsten Schmidt (PSI), Ming Shi (PSI), Grigory Smolentsev (PSI), Urs Staub (PSI), Dirk van der Marel (UniGE)

Summary and highlights: All subprojects with 14 new collaborations between computational and experimental partners have been started covering a broad range of topics related to VP1 and VP2. Among the first exciting results are the confirmation of a novel topological material, the gain of new insight into the relationship between thermodynamics, chemical stability and water splitting activity of Ru-based perovskites, and the input for refinements of Co_4O_4 catalytic cycles.

1 Main goals and achievements

The main goal of PP7 is to foster collaborations between theory and experiment for the experimental validation of results with an intense feedback loop for the design and discovery of novel materials and of materials displaying novel physics or improved properties or performance. For this a funding system for collaborative projects between computational and experimental groups consisting of funding for a postdoc has been implemented and two call for proposals launched. 14 projects have been granted all of which are now running.

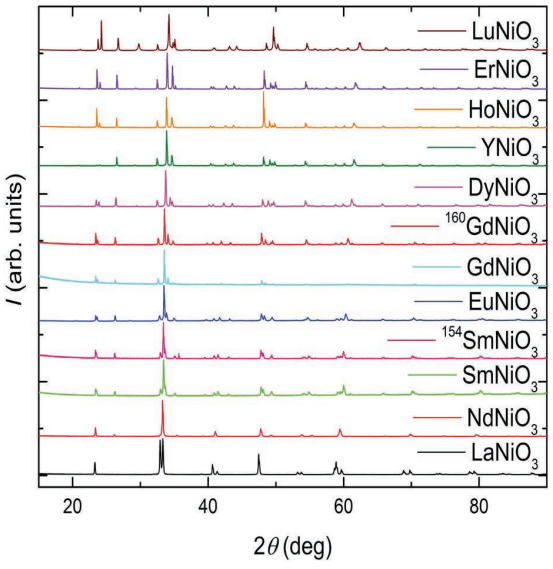

Figure 33: *Laboratory X-ray powder diffraction patterns of the $RNiO_3$ nickelates with R = La to Lu, including those synthesized with non-absorbing rare earth isotopes ^{154}Sm and ^{160}Gd.*

2 Scientific outputs

Most of the projects started in the middle of 2016, only some projects already started in 2015, therefore publishing joint results are just starting. Very nice example are the publication on oxygen evolution [147] (see Sec. 3.9), and the publication on Weyl nodes [5] (see Sec. 3.7).

3 Progress of the different efforts

The individual subprojects are at different stages, partly since they have been granted in the different calls for the second and third year. Postdocs have been hired, and sample growth and measurements have been started, as can be seen by the individual short reports.

VP1

3.1 $RNiO_3$ perovskites: exploring the boundary between localized and itinerant behavior

Marisa Medarde — PSI, Antoine Georges — UniGE, Nicola Spaldin — ETHZ, from Aug 2015, Dariusz Gawryluk

The last twelve months of the project were devoted to find the synthesis conditions for the different members of the $RNiO_3$ perovskite family (R = Y, Ho, Er, Tm, Yb and Lu). Besides large ($\sim$ 1 g) powder samples, 10-100 μm crystals could be prepared for the first time under high O_2 pressures (P_{max} = 2000 bar) for all members of the family. EDX and laboratory X-ray diffraction measurements performed on 20 μm $YNiO_3$ crystal confirmed the good quality and the absence of twins (Fig. 33). Next, neutron powder diffraction experiments

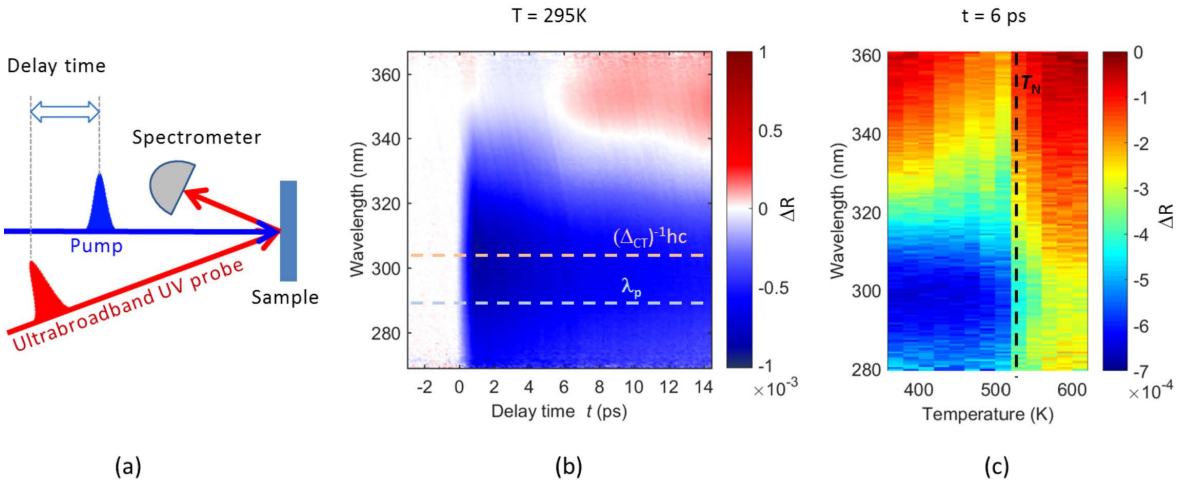

Figure 34: *(a) UV-pump/ultrabroadband-UV probe experiment. (b) Transient reflectivity change of bulk NiO deep in its antiferromagnetic phase after photoexcitation with a $\lambda_p = 290$ nm femtosecond pulse. The charge transfer gap of NiO $\Delta_{CT} = 4.1$ eV is indicated with an orange horizontal dashed line. (c) Reflectivity change measured at fixed pump-probe delay time of ~ 6 ps as a function of temperature.*

(R = La to Lu) and single crystal synchrotron X-ray diffraction (R = Y) were performed.
NMR and μSR measurements, suggested by our theory partners (Peil, Georges) and performed together with Mesot's group (ETHZ) could prove the existence of a new magnetic phase transition in $TlNiO_3$. Breathing modes linked to the metal-insulator transition (MIT) transition have been calculated by A. Hampel and C. Ederer and will be measured using inelastic X-ray scattering together with S. Rosenkranz (Argonne). Two publications about the comparison between the calculated and the observed distortion mode amplitudes determined from neutron diffraction are presently in preparation.
Collaborations with other groups for optical spectroscopy (van der Marel, UniGE), electric resistivity (Kenzelmann and Lortz, PSI + Uni Hong-Kong), Raman (Kamba, IOP Prague) and inelastic neutron scattering measurements (Petit, LLB Saclay) are ongoing.

3.2 Testing ultrafast processes in condensed matter

Urs Staub — PSI, Philipp Werner — UniFR, Nicola Spaldin — ETHZ, from Sep 2015, Michael Porer

Simulations of Hubbard-type models within the framework of dynamical mean-field theory have predicted a series of novel transient states in antiferromagnetic (AF) Mott insulating systems. Using ultrafast pump-probe techniques, we aim for first experimental tests of key predictions and to provide feedback for an improved and material specific modeling.
In a newly established collaboration with the group of M. Chergui (EPFL), we started an effort to test predictions on the relation between an antiferromagnetic spin background and the relaxation dynamics of photoexcited carriers in Mott-Hubbard insulators. We identified the antiferromagnetic Mott insulator NiO as promising reference system.
In our UV-pump/UV-probe experiment (Fig. 34a), a UV pump pulse centered around a wavelength of 290 nm generates a hot carrier population in bulk crystal of NiO via excitation across its charge transfer gap of $\sim$4.1 eV. An ultrabroadband UV-probe pulses with photon energies around the gap energy then probes the reflectivity change for a series of pump-probe delay times. By spectrally resolving the reflected probe pulses, we obtain 2D maps of the transient reflectivity change ΔR, as shown in Fig. 34b.
To study the influence of the magnetic order on the dynamics, we varied the temperature across the antiferromagnetic phase transition to $T = 550$ K. Up to now, we have collected data for $T = 295$ K and $T = 550$ K. In the present data, we could not yet observe a clear difference of the reflectivity dynamics for both temperatures on a timescale which could be related to carrier cooling effects (i.e. ≤ 100 fs). This is mainly due to the not optimal duration of the pump pulses, which was found to be higher than expected (i.e. > 100 fs) in a cross-correlation experiment. The group at EPFL has now upgraded the laser setup to enable optimum temporal compression of the pump pulses.

However, we observed a clear influence of the magnetism on the picosecond dynamics. Fig. 34c shows the spectral reflectivity change measured at a delay time of $\sim$ 6 ps as a function of temperature. It can be noted that ΔR at this delay time not only scales in amplitude with temperature, but also shows pronounced features around T_N, which are not present immediately after excitation (not shown). Since the ps dynamics can reflect several processes such as interband recombination or transient modifications of the band structure, a further understanding of the transient reflectivity changes needs further experiments and a more detailed data analysis (in progress).

3.3 Resonant inelastic X-ray scattering on thin films and oxide heterostructures for future mottronics and orbitronics

Thorsten Schmitt — PSI, Nicola Spaldin — ETHZ, from Jan 2016, Daniel McNally

We are studying early 3*d* transition metal-based films and heterostructures as a function of strain, dimensionality, and temperature combining X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS). We aim to understand the electronic structure changes in terms of 3*d* orbital reconstruction, 3*d* – O 2*p* covalency and degree of electronic localization when driving these systems across metal-insulator transitions.
During the past 10 months we have performed XAS and RIXS measurements on the $3d^1$ perovskite $CaVO_3$ as a function of film thickness and substrate. Our measurements reveal bandwidth reduction, increased localization and orbital reconstruction across the dimensionality driven metal-insulator transition (MIT). These results are important considering the wider net of 3*d* and 5*d* compounds that undergo MIT with reduced film thickness.
DFT+DMFT calculations predicted a MIT in $CaVO_3$ under tensile strain that may contribute to our measured MIT with reduced thickness, although we could not isolate the effect of strain for thicker films. We have provided this feedback to our VP1 theory colleagues. Next we plan to extend our tests of the predictive capabilities of DFT+DMFT for strongly correlated systems toward control of the MIT through superlattice construction.

3.4 Quest for the Higgs-mode in hexagonal manganites

Dirk van der Marel — UniGE, Nicola Spaldin — ETHZ, from May 2015 (matching), Adrien Stucky and Enrico Giannini

In this project an analogy is pursued between the Higgs mechanism of quantum field theory and an optical active mode existing in hexagonal manganites. Two types of hexagonal manganites ($ErMnO_3$ and $InMnO_3$) were investigated by optical spectroscopy with the aim of finding a Higgs mode.
It has been demonstrated theoretically by the Spaldin group [215, 155], that spontaneous symmetry breaking in $ErMnO_3$ and $InMnO_3$ crystals leads to a free-energy surface in the shape of Mexican hat, similar to the Higgs model. Associated to such a potential is an oscillation of the amplitude $|\Psi|$ perpendicular to the rim of the Mexican hat, which is equivalent to the Higgs mode. The optical study of crystals with this kind of structural symmetry breaking allows to confirm directly the existence of such a Higgs-like lattice vibration, and

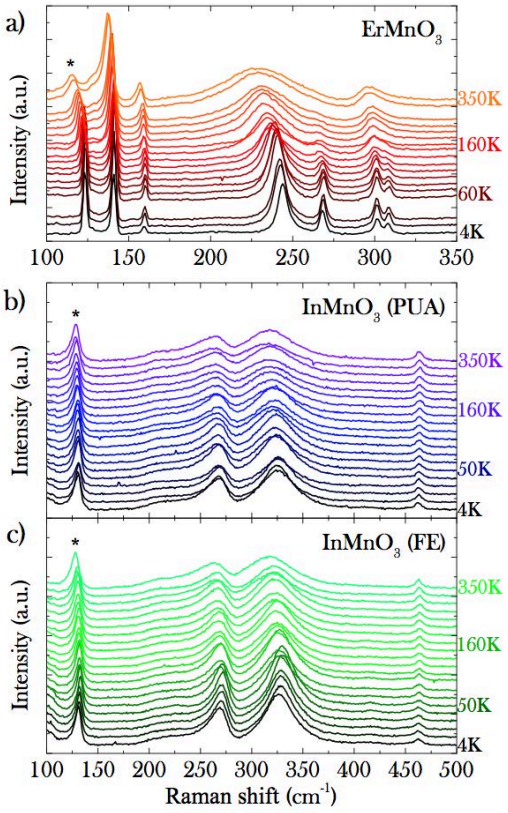

Figure 35: *Raman shift spectrum as a function of temperature from 4 K to 300 K in steps of 10/20/25 K. (a) $ErMnO_3$, (b) $InMnO_3$ (PUA) and (c) $InMnO_3$ (FE).*

determine its energy $\hbar\omega_H$.
Fig. 35 presents the Raman spectra of three $X\mathrm{MnO_3}$ crystals. The stars indicate the Higgs modes according to the theoretical predictions. The frequency shift of the Raman active mode and the broadening as a function of increasing temperature are due to the anharmonicity implicit in a Mexican hat potential.
As of Jan 2017 further low frequency and low temperature Raman experiments will be carried out with the aim to explore the collective modes related to Goldstone degree of freedom along the rim of the hat. Theoretical modeling of the anharmonicity, the effects of zero point fluctuations and coupling between Higgs and Goldstone modes are planned for the 4th year.

3.5 Single-band Hubbard model in new fluorides

Christian Rüegg — PSI, Nicola Spaldin — ETHZ, Thomas Schulthess — ETHZ, Matthias Troyer — ETHZ, from May 2016, Fan Xiao

The Hubbard Hamiltonian is arguably the simplest effective model describing electrons, which both move with hopping amplitude t and interact via the Hubbard parameter U. A well-known limit is the Heisenberg Hamiltonian for large ratio U/t of interacting localized spins. A solution of the complete Hubbard Hamiltonian has been a holy grail for decades in both theoretical physics and for large-scale numerical simulations. Here we are using an alternative, experimental approach. Following a proposal by the MARVEL group leaders Spaldin, Schulthess and Troyer [19], we synthesized a model material.
We will experimentally verify the predictions from the *ab initio* methods concerning the structural and electronic properties specifically of the new fluoride $\mathrm{NaCuF_3}$. During the past six months we have made significant progress towards the goals of this project. First, we have successfully synthesized $\mathrm{NaCuF_3}$ in the solid chemistry lab at University of Bern, both in powder and single crystal form. Fig. 36 shows the first single crystals of the material. Second, X-ray powder diffraction measurements have been carried out to investigate the atomic structure. We are currently planning the first neutron diffraction and spectroscopy experiments on the material at the Rutherford Appleton Laboratory (UK) and at the Swiss Spallation Neutron Source SINQ at PSI. Once the structural and spectroscopic properties are fully characterized, the results will be fed back to the theory and computational collaborators within MARVEL to model the material and identify possible, relevant corrections to the initial genuine Hubbard Hamiltonian.

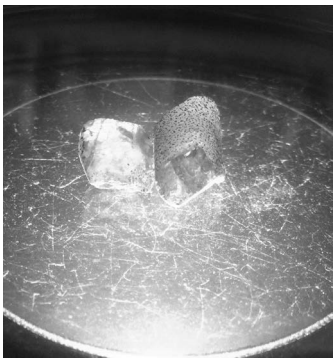

Figure 36: *$\mathrm{NaCuF_3}$ single crystals (volume 1 cm^3) synthesized at the University of Bern.*

3.6 Atomic-scale investigation of ferroelectric properties of Aurivillius phase $\mathrm{Bi_5FeTi_3O_{15}}$

Marta Rossell — Empa, Claude Ederer and Nicola Spaldin — ETHZ, from June 2016, Marco Campanini

The effect of doping and epitaxial strain on the structure and the ferroelectric properties of the Aurivillius phase have been predicted by *ab initio* calculations [216, 217]. The experimental characterization of these systems is very challenging, being the typical atomic displacements involved in the polar distortions in the range $10 - 50$ pm [218, 219].
Probe-corrected scanning transmission electron microscopy (STEM) is a very powerful technique capable of performing the above-mentioned investigations at sub-Ångstrom resolution, thanks to different imaging techniques with different chemical sensitivity — e.g. high angle annular dark field (HAADF) and annular bright field (ABF), that give access to both heavy and light atomic columns — and simultaneous spectroscopic analysis — i.e. energy dispersive X-ray spectrometry (EDXS) and electron energy loss spectroscopy (EELS).
Combining the HAADF and ABF signals, the accurate positions of all the different atomic species in the structure are precisely measured fitting the peaks of the images with 2D asymmetric gaussians [220]. The polarization at the atomic scale can therefore be computed as the displacement of the *B* cation with respect to the center of mass of the cell or, alternatively, by the offset between the centers of mass of the cationic and anionic charges. As an example, a map of the local polarization in the strain-free Aurivillius phase of $\mathrm{Bi_5FeTi_3O_{15}}$ is reported in

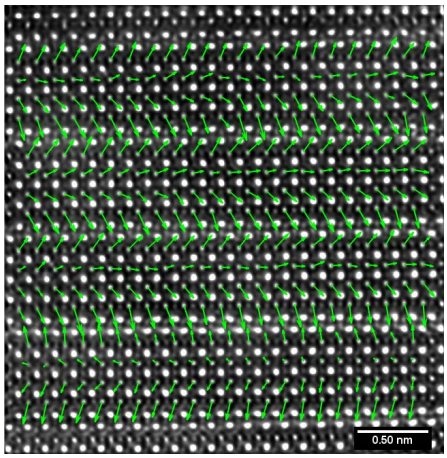

Figure 37: *Polarization map of the strain-free Aurivillius phase superimposed to the STEM-HAADF image.*

Fig. 37, as obtained from the displacements of the *B* cations. The next step of our work will involve the characterization of the strained and doped Aurivillius phase to verify if the epitaxial strain is able to induce an ordering of the dopants as predicted by DFT calculations and understand its potential effects on the local polarization. This further study will be carried out by combining the developed algorithm with atomically-resolved spectroscopies.

3.7 ARPES studies of novel topological materials

Ming Shi — PSI, Oleg Yazyev — EPFL, Matthias Troyer — ETHZ, from Sep 2016, Mengyu Yao

We aim at realizing novel topological materials, as well as investigating electronic structure evolution in the transition from a trivial phase to a topological non-trivial phase, by joint experimental and theoretical efforts. Using angle-resolved photoemission spectroscopy (ARPES) we focus on revealing the essence of the bulk electronic structure of various topological materials candidates, as well as identifying their manifestations on surfaces and/or interfaces.

In 2016, combining ARPES and first-principles calculations, (1) we revealed that TaP is a Weyl semimetal with only a single type of Weyl fermions, topologically distinguished from TaAs where two types of Weyl fermions contribute to the low-energy physical properties [5]. The simple Weyl fermions in TaP are not only of fundamental interests but also of great potential for future applications. Fermi arcs on the Ta-terminated surface were also observed, which appear in a different pattern from that on the As-termination in TaAs and NbAs; and (2) we identified topological Fermi arc states and the bulk bands of $MoTe_2$, and established that $MoTe_2$ is a type-II Weyl semimetal as it is shown from calculations [21]. In addition, we wrote a topical review article to summarize what have been achieved in the studies of topological Kondo insulators by using ARPES so far [148].

In the coming year we shall continue to carry out the following activities: (1) experimentally realize novel topological materials, e.g. magnetic Weyl semi-metals and/or nodal-chain metals [3]; (2) resolve the puzzle of the different magneto-transport properties observed in TaAs, TaP and NbP, in which the similar Fermi arc states were observed; and (3) study the possible topological phase transition from CaAgP to CaAgAs (a nodal-line semi-metal candidate).

VP2

3.8 Oxynitrides as photoanodes for visible light water splitting

Thomas Lippert — PSI, Nicola Marzari — EPFL, from Jun 2015, Wenping Si

This project aims at discovering novel perovskite oxynitride materials for solar light water splitting following the calculations of our collaborator Ivano Castelli. The correlations between photoelectrochemical performances and different surface orientations of $LaTiO_2N$ thin films deposited by pulsed laser deposition have been investigated. On the other hand, we have investigated the effects of various co-catalysts on the photoelectrochemical performances of the $LaTaON_2$ powders (Fig. 38). Y-Ta-O-N system, as predicted by calculation, has also been studied.

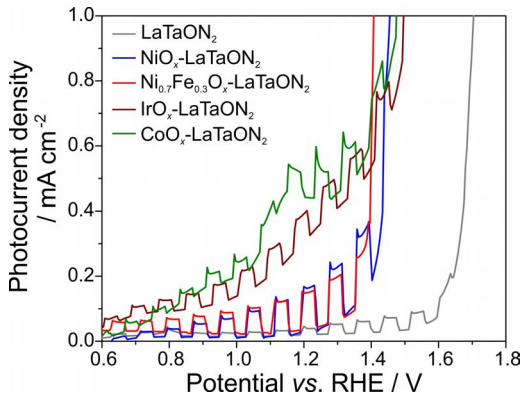

Figure 38: *Co-catalysts loaded on $LaTaON_2$ photoanode to improve the photoelectrochemical performance.*

Through the thermal ammonolysis of $YTaO_4$, pyrochlore $Y_2Ta_2O_5N_2$, fluorite $YTa(O,N,\square)_4$ and perovskite $YTaON_2$ all appeared at various temperature, ammonia flow and treatment time.

3.9 Unraveling thermodynamics, stability, and oxygen evolution activity of strontium ruthenium perovskites

Thomas Schmidt — PSI, Nicola Marzari — EPFL, from Aug 2015, Daniel Abbott

The main goal of the present project is to provide a fundamental understanding of the water splitting reaction on perovskite electrocatalysts, which could represent a breakthrough in the development of cost-effective water electrolyzers. The novelty of this research project lies in the use of operando X-ray absorption spectroscopy (XAS) which can provide dynamics of the electrocatalyst electronic and local structure. The experimental studies are combined with DFT simulations performed by the Marzari group at EPFL.

In a first approach we have selected $SrRuO_3$ as a model perovskite system. Experimental results and DFT calculations have both shown that this structure is not thermodynamically stable under water splitting conditions. Therefore, the high activity of this material measured in other reports is rather due to sample dissolution than to a truly water splitting reaction. A manuscript collecting all the experimental and DFT results is currently in preparation. This study provides a new insight into the relationship between thermodynamics, (electro)chemical stability and water splitting activity of Ru-based perovskites.

We are now moving towards more stable perovskite structures, still displaying high water splitting activity, i.e. the double perovskite family.

In the described experiments the water splitting activity is determined using a basic electrolyte. However, since now the industrial interest is moving towards water splitting catalysts operating in quasi-neutral environment, a new project goal will be the understanding of the water splitting mechanism as a function of the electrolyte pH value.

One joined publications appeared in *Chemistry of Materials* [147] and another one is in preparation.

3.10 *In situ* structural and electrochemical characterization of phase transformations at oxide-liquid interface

Claudia Cancellieri — Empa, Alfredo Pasquarello — EPFL, Daniele Passerone — Empa, form Jan 2016, Fabio Evangelisti

Our project addresses the microstructure-property relationships of defective functional oxides as function of both the growth and the environmental exposure conditions. As a first step, the structure and electronic properties of amorphous Al_2O_3, as grown by anodization at different anodization potentials V, were investigated by experiment and theory [149]. The thus-obtained barrier-type Al_2O_3 layers were systematically investigated by a combinatorial experimental approach using spectroscopic ellipsometry, X-ray photoelectron spectroscopy (XPS), SEM, TEM, electrochemical impedance spectroscopy (EIS) and scanning kelvin probe force microscopy (SKPFM). The layer thickness linearly increases with increasing V in the range from 20 nm to 350 nm and they are fully amorphous by XRD and TEM. The experimental findings in combination with DFT modeling of the amorphous structure and related electronic properties could disclose the relationships between the dielectric response, the oxide density and the anodization potential. Two distinct growth regimes were revealed, as associated with the formation of low density oxides at $V < 100$ V and high density oxides at $100 \leq V < 250$ V (corresponding to thicknesses > 120 nm) (Fig. 39). With increasing anodization potential in the range of $100 < V < 250$ V, the overall density of the grown oxide layers increases, but at the same time shallow pores and roughness start to appear on the oxide surface. The next important step (in close-collaboration between the experimentalists and modelers) will be to identify the structural defects in the amorphous oxide structure, which govern the electronic properties. A MARVEL internal collaboration is started with D. Pergolesi and F. Haydous at PSI for in depth-spectroscopic measurements.

3.11 XANES characterization of $Co_4^{II}O_4$ water oxidation catalyst. Experimental and calculated results comparison

Grigory Smolentsev — PSI, Jürg Hutter — UZH, from Apr 2016, Nicoló Azzaroli

Artificial photosynthesis is a promising solution to face world clean energy demand. We investigate molecular Co_4O_4 catalysts for water

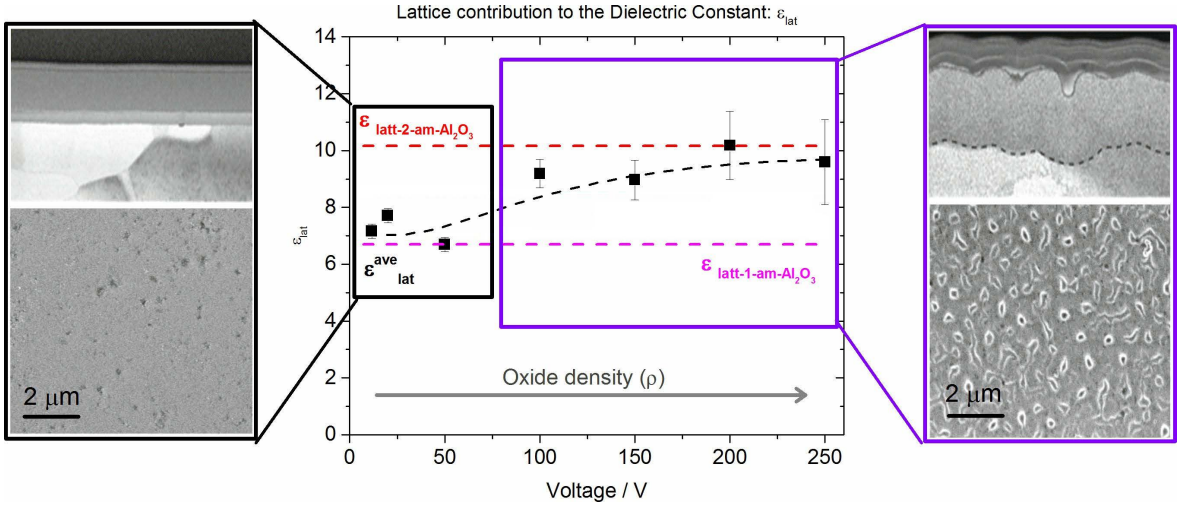

Figure 39: *Schematic summary of the first year MARVEL activity. Al anodic barrier oxides dielectric and morphological properties were investigated as a function of the growth voltage. The experimental dielectric constants are compared to the ϵ values calculated by DFT for 2 different amorphous densities: 1-am of 3.31 g/cm^3 and 2-am of 4.1 g/cm^3. Two different regimes are clearly identified.*

splitting [164]. The goal of the project is to clarify the reaction mechanism by determination of local electronic and atomic structure of different states of the catalyst formed during the reaction. Theoretical models of the catalytic cycle are based on the assumption that in the resting state all Co atoms have 2+ oxidation state [40]. In these models, one or two Co atoms change the oxidation state during the catalytic cycle. During *in situ* time-resolved X-ray absorption near edge structure (XANES) experiment, we have found the transition from high spin Co(II) to low spin Co(III) state for the majority of Co atoms that occurs during the first minute of the reaction. Therefore the resting state of the catalyst during water splitting has all four Co centers in the low spin Co(III) state (Fig. 40). Based on this new data the model of the catalytic cycle is under revision. Calculations of XANES for the structural model of Co_4^{III} state obtained by theory partners of the project agree with the experimental spectrum of the catalytic resting state. Further experiments to characterize intermediate states of the catalyst are in progress. These results represent the first cycle of the feedback loop between theory and experiment which is crucial to draw a correct picture of the catalytic mechanism.

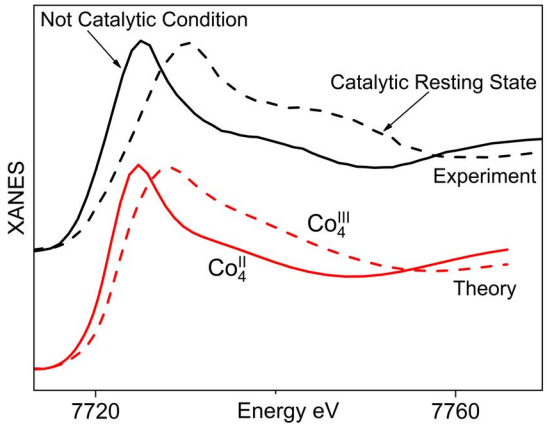

Figure 40: *Co K-edge X-ray absorption spectra of Co_4O_4 cubane catalysts.*

3.12 Colloidal nanocrystals as model systems to uncover structure/properties relations in CO_2 electroreduction

Raffaella Buonsanti — EPFL, Nicola Marzari — EPFL, from May 2016, Jianfeng Huang

During the first six months of the project progress has been made along two research directions:

a) *The study of the morphological evolution of Cu nanocrystals as electrocatalysts for CO_2 reduction* The structural reconstruction of the electrocatalysts during CO_2 reduction is of equal importance as the pristine morphology of the catalyst. How the reaction time affects the the morphology of nanocrystals with different sizes and shapes has been studied. It was found that smaller Cu nanocrystals (8 nm-spheres and 24 nm-cubes) decompose quickly into clusters within 3 h and the later then reconstruct into larger and shaped particles. By contrast, 44 nm-cubes are relatively more stable. While a degradation that produces clusters surrounding the nanocrystals takes place slowly, they preserve the cubic shape even af-

ter 12 h. The theoretical validation of the morphological evolution and the correlation of the morphological changes with the electrochemical activity and selectivity are in progress.

b) *The development of the synthesis of Ag-Cu nanocrystals with controlled morphology and composition* Alloying Cu with Ag is a promising strategy to create efficient electrocatalysts for electrochemical CO_2 reduction, because it potentially breaks the "scaling relationship" of the intermediates formed in the reaction pathway from CO_2 to hydrocarbons. By manipulating the co-deposition of Cu and Ag atoms on pre-synthesized Ag cubes, we have developed Ag-Cu alloyed nanooctahedrons that are bound with {111} planes and have a defined compositional percentage of each element. Future efforts will be devoted to the measurements of the electrocatalytic activities of these nanocrystals for CO_2 reduction and a theoretical corroboration on the alloying effects on the electrochemical CO_2 reduction

3.13 The search for new proton conductors: high-throughput screening and experimental synthesis and characterization

Daniele Pergolesi — PSI, Nicola Marzari — EPFL, from May 2016, Elisa Gilardi

The aim of this project, is to compute and synthesize novel proton conductors. The expected properties of the materials are good proton conductivity and chemical stability in the SOFCs (solid oxide fuel cells) operating conditions. Computational screening focused on the perovskite structures. The main criteria chosen for the screening are the material stability and mobility of the charge carriers. Mobility of the protonic charge carriers is studied by computation of single particle diffusion coefficient by first principle MD under DFT approximation. A constant loop between theoretical calculations and experimental validations is scheduled.
The study of reference materials as ceramic pellets and thin films is now ongoing (Fig. 41). In particular we focused on the characterization of structural and electrical properties of barium zirconate doped with Yb, Gd and Y to investigate the effect of different dopants and strain on the proton conductivity. This work widens the previous study of the effect of the ionic radii of the dopants on the structural and electrical properties of doped barium zirconate [151].

3.14 Experimental design and computational refinement of novel phosphine-functionalised metal-organic frameworks as efficient hydroformylation catalysts of olefines

Marco Ranocchiari — PSI and Wendy Queen — EPFL, Berend Smit — EPFL, from Jul 2016, Gerald Bauer

The challenge in this project is the low stability and the low regioselectivity of the Co-phosphine complexes under hydroformylation conditions [221, 222]. It was shown that the complex stability can be enhanced with increased steric hinderance of the ligands. Metal-organic frameworks (MOFs) are a solution to this problem due to their crystalline and porous structure, high surface area, tailored pore surface and thermal stability [223].
As a proof of concept we chose a UMCM-1 structure (Fig. 42) because (1) the known crystal structure facilitates the computational in-

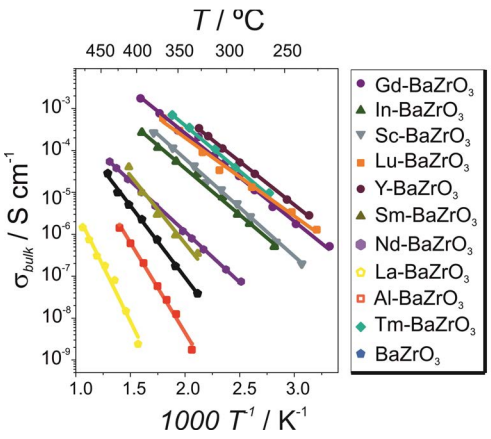

Figure 41: *Temperature dependence of the bulk conductivity of $BaZrO_3$ doped with different trivalent dopants.*

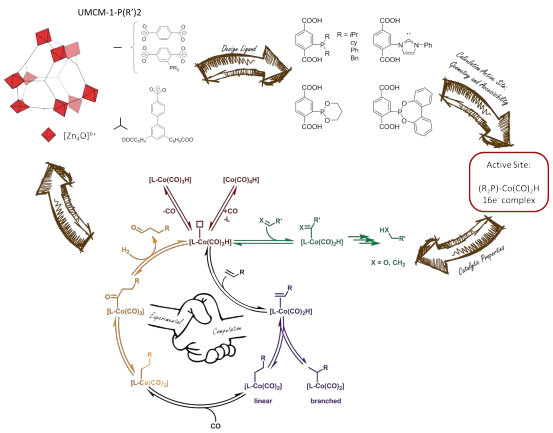

Figure 42: *Flow scheme of the iterative optimisation of the cobalt catalysed hydroformylation by cobalt doped MOFs.*

vestigations, (2) its large pores, (3) the featured terephthalic acid linker, which can be easily derivatized with phosphines exhibiting different electronic properties. These phosphine derivatives will act as coordination site. We commenced the synthesis of the different phosphino-terephtalic acids (Fig. 42). In parallel first-principles DFT simulations have been performed to optimise the ground-state geometry of the functionalized UMCM-1. DFT calculations will be done to predict the performance of each ligand under reaction conditions. Finally, classic Monte Carlo and molecular dynamic simulations will be performed to study the active site and diffusion inside of the MOF.
Iterations of this process with different MOFs and/or different phosphine linkers will help us to fine-tune the catalytic performance of the Co-catalyst.

4 Contribution to overall goals and initial proposal

In the initial proposal, a wide range of possible topics and techniques have been addressed in order to be able to react on the developments on the computational side. The aim was to foster collaboration for the design and discovery of novel materials and of materials displaying novel physics or improved properties or performance. All projects are contributing to these aims. The topics of most individual subprojects are in the frame of the initial proposal, only the topic of metal-organic frameworks (MOF) was added during the evolution of MARVEL.

5 Collaborative and interdisciplinary components

Through this platform, 14 new collaborations have been started, partly including more than two partners. The theory and experimental partners of the different sub-projects meet regularly to discuss the progress of the projects. For sample synthesis and characterization sometimes groups outside MARVEL are involved. In addition to the granted projects the general interaction between the computational partners and the experimental groups has been increased.

4.2 New projects

As a follow-up to the review panel's recommendations, we recovered 1 M CHF in funding to the launch of new projects, with the target that they should all be collaborative in nature, they should be led by junior or new personnel, and they should build synergies and expertise in preparation for phase 2. The 6 projects below were selected for start in January 2017, and one of them sees the inclusion of a new MARVEL group leader (SNSF assistant professor Ulrich Aschauer); 2 projects will be added in May 2017, to include two new MARVEL group leaders (tenure-track assistant professor Martin Jaggi, and full professor William Curtin). The 6 projects for January 2017 are:

- Ulrich Aschauer (UniBe), "Stoichiometry as a materials-design parameter"; in collaboration with Nicola Spaldin and Alfredo Pasquarello.
- Michele Ceriotti (EPFL) "QMAT-x: a reference dataset for machine learning of materials properties"; in collaboration with Anatole von Lilienfeld.
- Daniele Passerone (Empa), "AiiDA workflows oriented to low-dimensional nanostructures and AiiDA CP2K plugins"; in collaboration with Nicola Marzari.
- Berend Smit (EPFL), "Bringing the nanoporous genome in the materials cloud"; in collaboration with Giovanni Pizzi.
- Anatole von Lilienfeld (UniBas), "Machine learning models for the computational design of catalysts"; in collaboration with Clémence Corminboeuf.
- Oleg Yazyev (EPFL), "Computational workflow and data infrastructure for high-throughput search of novel materials"; in collaboration with Nicola Marzari.

All the agility grants allocated for years 1-2 were renewed with the exception of Wanda Andreoni, that since retired from EPFL. Joost VandeVondele's project stopped end of October 2016, when he left ETHZ for CSCS.

Year 3 saw, as planned, the start of the second series of seven experimental projects planned for the second call of PP7.

5 Knowledge and technology transfer

Knowledge and technology transfer in MARVEL occurs at different levels: knowledge transfer takes place in the dissemination of open-source simulation codes, training in the use of those codes and of the newly developed materials informatics framework, in the sharing of all results from materials simulations, and verification and validation of the calculations. The technology transfer activities focused this year on approaching companies in five industrial sectors of interest, while developing list of target companies in Switzerland and abroad, and led to numerous meetings with companies and visits on campus. By building an industrial community around MARVEL, and with the help of an industrial advisory board, and enhanced visibility, we aim to nucleate new collaborations and projects with the industrial sector.

Software

AiiDA

The open source platform AiiDA (www.aiida.net) is presented in detail in the scientific report on PP6. Two major releases, v.0.6.0 on Mar 1 and v.0.7.0 on Aug 10, 2016, took place last year with all recent updates and new functionalities. Four AiiDA tutorials were organized, one in Kyoto, two in Trieste and one at EPFL, and an additional one will take place at EPFL in May 2017. Since the beginning of MARVEL, these summed up to 290 attendees — users and developers. Some tutorials have been co-sponsored by centers outside MARVEL, such as the MaX CoE, Psi-k, CECAM, ICTP. In particular the last 2 tutorials, held at EPFL and in Trieste, were recorded and will be made available online. 15 developers contributed to improve AiiDA during one coding week in the Swiss Alps in Dec 2016. Half the participants were core AiiDA developers, the other being programmers motivated to contribute to AiiDA. In semester projects, a group of 8 computer science students from Prof. Koch's "Big Data" course investigated possible extensions of AiiDA using other SQL and NoSQL databases and one of them continued putting the grounds for the multi-backend support. Multiple efforts, including the various code plugin developments taking place in multiple groups, are constantly coordinated, with biweekly meetings with the full AiiDA team, including the team at Bosch RTC in the USA. We are also taking care of the coordination with various computer centers (CSCS, CINECA, Jülich, etc.) toward the deployment of AiiDA directly on the supercomputers.

Materials Cloud

Materials Cloud is a web portal (materials-cloud.org) with a major aim at knowledge transfer. This portal, described in more detail in the scientific report on PP6, provides an online environment integrating the various resources needed by computational material scientists to pursue their research objectives. These are grouped into four categories: *Learn*, *Work*, *Discover*, and *Explore*, the first three being specifically aimed at the knowledge transfer. The purpose of *Learn* is to make educational resources such as video lectures, tutorials, and course notes freely available for those who want to learn material science to various degrees. Present resources include a Quantum-ESPRESSO school and an AiiDA tutorial. *Discover* is a collector of curated datasets of materials properties contributed by the researchers who want to disseminate their results. Two projects — Standard Solid State Pseudopotential and SketchMaps — are already published on *Discover* and the inclusion of 4 more projects is scheduled. Finally, the *Work* section will serve as a platform hosting the open-source efforts developed within MARVEL — such as AiiDA workflows and plugins — freely reusable by the academics.

H2020 Activities: MaX CoE, NFFA, and EMMC CSA

The H2020 MaX Centre of Excellence for e-Infrastructure has the shared goal of developing codes and tools for "Materials Design at the eXascale"; MARVEL is part of it through Marzari and Schulthess, and it provides a key network where other groups work on the AiiDA platform (the developers of FLEUR, Yambo, and SIESTA) and the five supercomputer centers involved (CINECA, CSCS, Jülich, BSC, and KTH) plan joint efforts, in which the mirroring at CINECA of the CSCS Materials Cloud services will be the first outcome. The H2020 NFFA (Nanoscience Foundries and Fine Analysis) is an effort to provide experimental and computational services to the community at large, and Marzari is part of the Theory and Simulation installation — in the future we plan to deploy software-as-a-service solutions, modeled around the Materials Cloud. In addition a JRA (Joint Research Activity) is dedicated to developing standards for data and metadata for experimental and computational efforts, with close interactions between the Materials Cloud team and experimental efforts at the Rutherford Appleton Laboratory and the Karlsruhe Institute of Technology. Finally, the H2020 EMMC CSA (Coordination and Support Action for the European Materials Modeling Council) is an effort to collect and compile input from all stakeholders on the future needs and directions of materials modeling in Europe, and to involve all stakeholders in model development, interoperability and metadata, best practices and articulating economic and business impacts, with EPFL/MARVEL as one of the 15 partners.

New open source codes: Z2Pack and ENVIRON

Z2Pack (http://z2pack.ethz.ch) is a a tool to calculate topological invariants for real materials that was developed by the groups of Troyer and Yazyev [20]. A public release is available. The code can identify topological phases from $\mathbf{k} \cdot \mathbf{p}$ or tight-binding models, or directly from some first-principles codes, and it benefit from close integration with the WANNIER90 codes developed by Marzari and collaborators. ENVIRON (http://www.quantum-environment.org/ is a module to perform first-principles calculations under realistic electrochemical conditions (i.e. in the presence of a solvent, an electrolyte, an applied electrochemical potential). Originally developed in the Marzari group, it has now developed in close collaboration with the Goedecker group, and discussed also in HP3.

Hardware

MARVEL owns a Cray XC30 cabinet at CSCS with 180 compute nodes, where each 24-core node is made of dual-socket Intel Xeon processors (Haswell 12 cores, E5-2680v3, 2.5 GHz). The collaboration agreement stipulated between ETHZ and MARVEL covered the timeframe from October 1, 2014 until September 30, 2018, and an in-kind support from ETHZ for electricity, cooling, maintenance, sysadmin, and data center/account management of 205'000 CHF/year. This collaboration agreement has now been extended till April 30, 2020, with ETHZ continuing its in-kind support till then. MARVEL has paid 200'000 CHF from its cash EPFL endowment for equipment to upgrade all the nodes to 36-core dual-socket nodes with Intel Xeon E5-2695v4, 2.10 GHz (18 cores, 64/128 GB RAM).

Conferences and collaborations

MARVEL members organized or co-organized more than 17 conferences and workshops, some of them being also sponsored by MARVEL. All are listed in the NIRA database and the list can be found on the website (nccr-marvel.ch/ctw).

A notable example where MARVEL figured prominently was the "Platform for Advances Scientific Computing PASC16" conference organized by CSCS on Jun 8 – 10, 2016 at EPFL, with Nicola Marzari as co-chair. An information booth promoting MARVEL activities together with a demonstration of the AiiDA platform was set-up by MARVEL management. Talks and posters were presented by MARVEL members from EPFL, IBM, UniBas and CSCS. Three mini-symposia were organized by MARVEL group leaders: Marzari organized the "Materials Design by High-Throughput Ab Initio Computing" session, Ceriotti the "From Materials' Data to Materials' Insight by Machine Learning" session, and Bekas the "HPC for the Big Data Era" session. Another one is the "Second Workshop of Ultrafast Dynamics in Strongly Correlated Systems", held on Oct 10 – 12, 2016 at PSI with Urs Staub and Philipp Werner as lead organizers. Other notable examples were the CECAM workshop on "Exploring chemical space with machine learning" organized in Zurich on May 30 – Jun 3, 2016 by Anatole von Lilienfeld, that included 3 invited speakers plus 6 participants from MARVEL.

and the CECAM/Psi-k School on "Path Integral Quantum Mechanics: Theory, Simulation and Application", co-organized by Michele Ceriotti in Lausanne on Jun 13 – 17, 2016.
The ECAM "WANNIER90 Software Development Workshop" held on Sep 12 – 16, 2016 in San Sebastian, Spain was also co-sponsored and supported by MARVEL. The aim of the workshop was to share recent developments related to the generation and use of maximally-localized Wannier functions and to either implement these developments in, or interface them to, the WANNIER90 code. 29 participants from all over the world, including several members of the Marzari, Troyer, and Hutter groups attended this "coding week". The model was so successful that it was reproduced, equally successfully, with the AiiDA "coding week in the Alps" mentioned above. Another important event was the "Open Databases Integration for Materials Design" Workshop organized by the Lorentz Center on Oct 24 – 28, 2016 in Leiden, The Netherlands, that had as its goal the conception and development of a common API (the Optimade API) able to interrogate all current materials databases with the same syntax - a paper and standard are currently been written, and participation of all major European and US players assured broad support from the beginning. Last, the Parrinello group is organizing a school on variationally enhanced sampling, a method developed within MARVEL. The school, sponsored by MARVEL, will take place at USI on Feb 14 – 17, 2017 (sites.google.com/site/vesschool2017).

Technology transfer

In 2015, we prepared a portfolio of MARVEL research topics of interest for companies, and defined five industrial sectors to target.

- Energy harvesting, conversion and storage.
- Information-and-communication technologies.
- Organic crystals/pharmaceuticals compounds.
- Catalysis and chemical synthesis.
- Watch-making industry.

In 2016, we approached companies from these five sectors, and started to create a list of "companies of interest" in Switzerland and also abroad. The final aim is to establish an industrial community around MARVEL and to increase the number of collaborations. The same line will be maintained for year 4. The tech transfer officer has visited PSI and Empa, to better know experimental partners and their work. Events dedicated to companies will be organized with CCMX and Empa-Akademie in 2017.

Creation of an industrial community

Quantum molecular simulation is a fast-evolving field in academic research and a large community exists. In the industrial R&D, the experimental approach is by far the most largely used. Most of SMEs and even some large companies active in materials science are not aware of this emerging field and do not always understand what to expect. Some large international companies, with large R&D centers, have dedicated teams to "advanced modeling of materials". For this reason, our efforts will be mainly directed towards large Swiss companies and, in parallel, large foreign companies investing already in the modeling approach beside the classical experimental approach.

Actions to increase the awareness/promotion

- CCMX Annual Meeting, May 11, 2016, Bern: poster presenting MARVEL.
- STI Industry Day, May 18, 2016, EPFL: presentation of MARVEL profile to get one-to-one meetings.
- World Materials Forum, Jun 9 – 10, 2016, Nancy (FR): participation & networking. Event gathering large companies active in materials (Solvay, Saint-Gobain, Mitsubishi, Morgan Advanced Materials).
- Awareness emails to target people in companies active in materials. A database of companies in contact with MARVEL is being elaborated with the aim to share specific news or to inform about activities.

Company visits

Four large company visits have been organized at EPFL, among them two Japanese, one US and one European. These consist of half-day visits with presentations of labs affiliated to MARVEL.

On-going discussions/negotiations

In 2016, a total of 24 companies has been in contact with MARVEL at different levels, as compared to 13 in 2015 (some being the same).

Sectors of activities:

	watch-making/ materials	energy	fine chemistry/pharma	electronics	others
2016	9	3	8	2	2
2015	3	2	4	2	2

Countries:

	CH	EU	USA	JP
2016	10	7	3	4
2015	5	5	1	2

Most promising interactions:

- 1 large European chemical company came twice and confirmed the interest to collaborate. A workshop with their experts in modeling will take place in spring to set up a collaboration.
- 1 pharma company had signed a non-disclosure agreement. After 2 meetings, the lab is now preparing an offer for a 6-month collaboration.
- 1 start-up is preparing a Commission of Technology and Innovation (CTI) proposal with Profs. von Lilienfeld and Marzari (18-month project).
- 4 companies which came for a visit are asking further information to identify possible collaborations and will come back for a second visit.
- 6 companies were met during an event and will receive the MARVEL newsletter in 2017.
- 7 companies received a first email of sensibilisation and will receive the MARVEL newsletter.

Signed collaborations

- 1 large company signed for an AiiDA licence with 2 years of technical support (2016 – 2017).
- 1 large company signed a 4-year research contract (2014 – 2018).
- 1 small company active in data-mining signed an agreement to give the Marzari group free access to data for research purpose.

6 Education and training

MARVEL continued focusing education and training activities on its PhD and postdoctoral researchers, and on the wider community, through training schools and workshops of broad, fundamental interest dedicated to researchers worldwide. MARVEL also provided sustained support activities in electronic-structure simulation and modeling in sub-saharan Africa. Regarding the younger generation, a camp for high school students is planed. A particular emphasis was put on junior scientists interactions and stimulation of new collaborations (junior retreat, junior seminars) to empower them to bring new ideas to the projects.

PhD students and postdoctoral researchers

In the MARVEL community

Junior retreat

The junior retreat, organized by young researchers, is a great opportunity to know other people working on similar or complementary projects. The informal atmosphere stimulates many academic and non-academic discussions, which have led to many new collaborations. The second edition took place on Jul 18 – 21, 2016 in Les Diablerets and was attended by 48 PhD students and postdocs working at EPFL, ETHZ, Empa, PSI, IBM, USI, UZH, UniGE, UniBas and UniFR (Fig. 1).

One of the key objectives was to promote creative collaboration. In addition to the usual social activities, participants were asked to prepare 8 mini-projects within designated groups of 6 and present them on the last day. The groups were pre-defined by the organizers to ensure that participants from the same research unit and/or MARVEL projects were in different groups to push the boundaries of current collaborations at the junior level. The outcomes were truly impressive, with proposals spanning across different fields of expertise, tackling the key environmental and societal challenges; these were then presented at the Review and Retreat in Sep 2016.

The third junior retreat is being organized by a new team of junior researchers and will take place in Jul 2017.

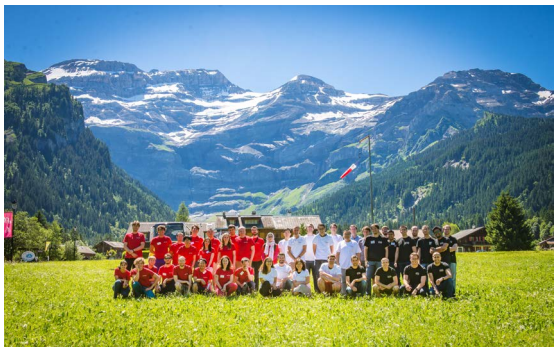

Figure 1: *Second MARVEL junior retreat on Jul 18 – 21, 2016, in Les Diablerets: group picture, the participants wearing their brand new MARVEL T-shirts.*

Participations to schools and tutorials

MARVEL continued supporting associated students to participate in various schools and workshops in the field of computational design and discovery of novel materials, or more generally in topics of current interest in theoretical condensed matter physics and materials science.

Education platform

Since last report, 2 more MARVEL distinguished lectures were made available through the MARVEL website on slideshot.epfl.ch/events/14 as well as a series of lectures on materials modeling from first principles based on Quantum-ESPRESSO slideshot.epfl.ch/events/16. All this material is being transferred on the materials cloud web portal in the *Learn* category, a permanent repository of educational resources, such as video lectures, tutorials, and associated

material on topics in electronic structure simulations.
Other MARVEL members also contributed educational material, such as the open-access lectures by Antoine Georges at the Collège de France (www.college-de-france.fr/site/antoine-georges/_audiovideos.htm), the lecture slides from the CECAM/Psi-k School on Path Integral Quantum Mechanics: Theory, Simulation and Application, organized by Michele Ceriotti (www.cecam.org/workshop-1314.html), and the Advanced Workshop on High-Performance and High-Throughput Materials Simulation using Quantum-ESPRESSO (indico.ictp.it/event/7921/). This material will also be made available through the Material Cloud *Learn* platform.

Outside MARVEL

Two core activities took place in collaboration with the International Centre for Theoretical Physics (ICTP) in Trieste: a tutorial on high-throughput computing, for 100+ students, organized in Jul 2016 as part of the 2-week "College on Multiscale Computational Modeling of Materials for Energy Applications" and a 2-week workshop on "High-Performance and High-Throughput Materials Simulations" in Jan 2017, in collaboration with the EU H2020 CoE MaX and with financial support by MARVEL.
The fourth African School on "Electronic Structure Methods and Applications", ASESMA-2016, took place at Accra, Ghana, on Jun 13 – 24, 2016. MARVEL sponsored this school, co-organized by the International Center for Theoretical Physics (ICTP) in Trieste. The NCCR was actively involved, with the participation of speakers and mentors/tutors members of MARVEL. MARVEL supported also the travel of 2 lecturers to Sudan for the Khartoum Workshop for the Advancements in Material Sciences (KWAMS'17), Jan 8 – 19, 2017. A highlight from one of the lecturers was seeing this year a beginner from the first Khartoum workshop in 2013 present her current PhD work at the University of Trieste in DFT.

At the level of Master students

The existing offer of computational classes at the Master and PhD level in the participating institutions is available from the MARVEL website. In particular, as mentioned in the last year report, new classes were introduced in the EPFL Section of Materials Science and Engineering in a synergetic approach that is particularly useful to computational materials science, as an initiative of Profs. Ceriotti and Marzari. The course "Molecular and Materials Modelling" offered for the last three years at the ETHZ Department of Materials by Joost VandeVondele and Daniele Passerone, is taught as of 2016 by Daniele Passerone and Carlo Pignedoli. Topics related to materials discovery with the computer will be enhanced, with targeted laboratory sessions involving simple but self-contained computer experiments.
IBM participated in the Academia Industry Modeling week organized by UZH and ETHZ on Nov 7 – 11, 2016. Students of various backgrounds worked on the characterization of ionic channels in solid-state structures.

For the younger generation

MARVEL high-school summer camp

The MARVEL education team is drafting plans for a 2-weeks summer camp for high-school students on computational science, to be held in Jul 2018. The EPFL high-performance computing team SCITAS has already agreed with enthusiasm to be involved in the organisation, and will provide both facilities and instructors for a few introductory lectures on scientific programming. Students taking part in the school will be invited to propose a scientific project, which will be discussed with the instructors and realized during the course of the camp. The school will be open to teenagers between 16 and 19 years old, corresponding to the last two years of high school. MARVEL will fund the organisation costs, transport for those who choose to go back to their homes every evening and accommodation for those who choose to stay overnight. As an equal opportunity action, a fixed quota of 50% girls will be imposed at registration. This first edition will also be used as a model to develop the same kind of camp in other Swiss linguistic regions.

Other activities

Antoine Georges participated in the "Speed Science" program of the French Academy of Sciences which brings about 80 high-school students to meet with members of the Academy from a range of different fields. The students discuss and ask questions about their interests in science as well as career opportunities in research. Vladimir Rybkin (VandeVondele's group) took part to the Annual Young Chemists School for 25 kids in Ivanovo, Russia.

7 Equal opportunities

In year 3, MARVEL has implemented and initiated new activities to advance equal opportunities, in line with its strategy. Established measures were continued, as was the exchange and cooperation with other NCCRs, the EPFL Equal Opportunities Office and the Science Outreach Department.

Strategy and recommendations from the site visit

Equal opportunities activities in year 3 have followed MARVEL's general equal opportunities strategy. MARVEL has also taken into account recommendations made during the 2016 site visit. Specifically,the inclusionof men into some parts of the equal opportunities activities in order to increase sensitivity and understanding with regard to supposedly innocuous actions that can create a non-inclusive community.

Numbers

Table 7.1 gives an overview of the number and share of women involved in MARVEL. The percentage of women rose in year 3, as of the 7 new experimental projects, 3 are headed by female group leaders.

	year 1		year 2		year 3	
	women	men	women	men	women	men
Group leaders	4 (17%)	20 (82%)	6 (18%)	27 (82%)	9 (22%)	32 (78%)
Postdocs	5 (11%)	40 (89%)	9 (13%)	59 (87%)	10 (13%)	67 (87%)
PhD	5 (24%)	16 (76%)	8 (22%)	29 (78%)	9 (19%)	38 (81%)

Table 7.1: *Number and share of women involved in MARVEL in years 1, 2 and 3.*

Raising gender awareness

Gender training

In order to contribute to an institutional culture favoring equal opportunities and preventing gender bias, the MARVEL executive committee has expressed a wish to train its members, from people with leadership functions to any new member, in gender and ethics. To this end, MARVEL has approached the EPFL Equal Opportunities Office, which has integrated in its 2017 – 2020 action plan an awareness training on issues around gender, diversity, harassment and respect. The idea is to prepare a training set in cooperation with the EPFL Research Office and the "Learning & Development" Unit at EPFL's HR department and test it on MARVEL members, before a more general implementation. These issues will be also addressed in the *welcome letter* prepared by the MARVEL management team.

Advance women scientists

INSPIRE fellowships

As a common initiative with the NCCR QSIT on "Quantum Science and Technology", MARVEL introduced the INSPIRE Potentials — MARVEL Master's Fellowships (nccr-marvel.ch/inspire) with the goal of empowering excellent female students to conduct a 6-month Master's thesis research in a computational laboratory belonging to MARVEL (Fig.1). This initiative seeks to increase the number of women researchers in the field of simulation science where they are underrepresented even at the undergraduate level and to provide an inspiring research environment for potential future PhD students and academics. The fellowships are advertised through the MARVEL group leaders, the gender equality offices of Swiss universities, targeted mailing lists, student fairs, etc.
Two calls took place in 2016, with 4 fellowships granted. The 4 students will begin their Mas-

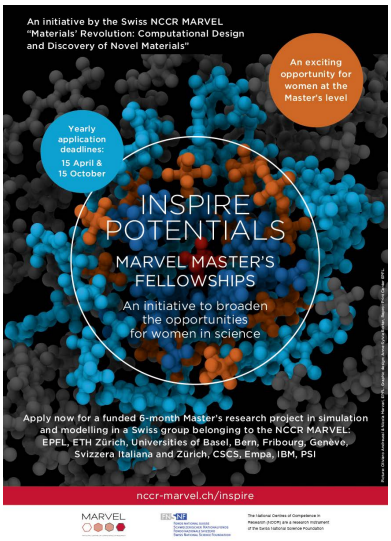

Figure 1: *Flyer advertising the INSPIRE Potentials — MARVEL Master's Fellowships.*

ter's research work between March and May 2017 in 4 different MARVEL groups chosen according to their list of preferred labs.

Lunch events

MARVEL has advertised lunch events and industry sight visits organized by the EPFL Equal Opportunities Office to its female PhD students and researchers. Seven events have been organized, with an attendance between 25 and 100 (over 55 participants on average). These events have provided opportunities to gain insight into different careers and to personally interact with role models from academia, industry, startups and entrepreneurship. Events in 2016 have been organized in cooperation with EPFL Innovation Park, female leaders from two startups, women professors, the EPFL-WISH Foundation, and companies such as Accenture, Google and Cisco.

Training, mentoring and coaching

MARVEL encourages its female PhD students and postdocs to take part in training, mentoring and coaching programs offered in the various institutions participating in MARVEL. All are advertised on the MARVEL website and MARVEL female students are regularly informed of their existence, or of the availability of new programs.

Recognition for female researchers' excellence

MARVEL distinguished lectures MARVEL has strived to increase the number of women invited for distinguished lectures. The 2 distinguished lectures in year 3 have been given by women. In total, 2 out of 7 distinguished lectures have been told by women, and a third one is planned for May 2017.

Prizes and distinctions Among the ongoing activities, MARVEL is creating a list of academic prizes in MARVEL related fields and/or for women researchers, to encourage NCCR women to apply for these prizes. In this context, it should be noted that several distinguished prizes have been awarded to female PIs and researchers. In year 3, Sandra Luber, postdoc in the group of Jürg Hutter, received the 2017 Clara Immerwahr Award, Ursula Röthlisberger received the Doron Prize 2016, and Nicola Spaldin received the 2017 L'Oréal-UNESCO for Women in Science Award.

Support work-life balance

MARVEL is committed to enhancing work-life balance for students and staff. Information about existing measures, daycare facilities and advice about work-life balance in the different institutions involved in MARVEL has been made available on the website and members of MARVEL are informed of their existence.

Actions for young girls

EPFL Science Outreach Department and Equal Opportunities Office work together with us to enhance the interest of young girls for STEM fields. With the support of MARVEL, specific activities in MARVEL related domains are developed. Through the organization of these activities, MARVEL acts to change behavior, decrease stereotypes and obstacles related to gender, support the development of knowledge and interest of young girls for MARVEL related fields, and increase their confidence in their capacities for STEM fields. These activities receive strong interest and are always fully booked.

Polythème workshop on materials

This workshop, developed especially for MARVEL, entitled *Diamant, alu, caoutchouc, ils sont fous ces matériaux !*, has as goal of helping 7 to 10 years old girls discover the world of material sciences. Different types of material and their properties are presented and the girls learn by performing simple hands-on experiments. The 4th and 5th editions took place on Sep 7, 14, 21, 2016 (Fig. 2 left) and on Jan 11, 18, 25, 2017. A

Figure 2: *Workshops and camp for young girls at EPFL. From left to right: workshop* Diamant, alu, caoutchouc, ils sont fous ces matériaux !*; summer camp* Matériaux super géniaux*; summer camp in chemistry; mathematics workshop* Maths en jeu.

woman scientist conducted the workshop and acted as a role model.

Summer camp Matériaux super géniaux

The second edition of this scientific camp for 11 to 13 years old girls was organized in Aug 2016 (Fig. 2 center-left). Besides hands-on experiments and theoretical explanations, the girls could discover the research running in different labs of MARVEL and prepared a presentation given in front of their friends and families on the subjects they learned in these labs. The Aug 2017 camp is already fully booked.

Chemistry summer camp

This 5-day camp was organized in a real chemistry lab in Aug 2016 for 11 to 13 years old girls and boys with a 50% quota for girls (Fig. 2 center-right). Various experiments allow children to discover different fields of chemistry and chemical engineering and the usefulness of these fields. Children visit labs and discuss with researchers who act as role models.

Mathematics workshops Maths en jeu

These workshops are organized thanks to the joint funding of MARVEL and the EPFL Science Outreach Department. Workshops at 4 different levels were successfully organized from Mar to Jun and from Sep to Dec 2016 (Fig. 2 right). Some workshops were girls-only and some others for girls and boys (with 50% girls). The ages were 7 to 13.

8 Communication

In its third year, MARVEL continued implementing its communication strategy. The website was regularly updated. Several types of meetings were organized to strengthen internal communication and to energize the MARVEL community and network. MARVEL had the opportunity to team up with external events to open up its communication to scientists in the domain of material simulation at the national and international level, industrial partners, media and the general public.

Internal and external communication

1 Website and newsletter

The website nccr-marvel.ch serves two main communication purposes: internal and external communications on MARVEL. It is regularly updated with pertinent information on projects, people, events and news for ensuring smooth internal communication. A tool-kit for editing a newsletter from website items started being implemented in Jan 2017. The first internal newsletter release is planned for Feb 2017, with the aim to foster transversal communication between the different research groups in MARVEL, as well as to, in a second stage, open up to an outside audience, including industry. A first issue for an external audience is planned before end of year 3. In the meantime, emails covering the events, seminars and courses organized by MARVEL members/management in Switzerland and abroad are regularly sent to the whole community. These emails also include congratulations on awards won by MARVEL members.

2 MARVEL distinguished lectures

MARVEL continued inviting worldwide recognized experts in computational materials science to present a "MARVEL distinguished lecture". This year, 2 lectures were organized at EPFL, gathering a public of 40 to 50 people per event. A specific effort was made to invite world renown women.

- On Oct 26, 2016, Prof. Clare P. Grey (Univ. Cambridge, UK) gave the lecture "Structure and dynamics in batteries, supercapacitors and fuel cell materials: application of new experimental and theoretical approaches to study function".
- On Dec 20, 2016, Prof. Laura Gagliardi (Univ. Minnesota, USA) presented on "Homogenous and heterogeneous catalysis: two challenges for modern quantum chemistry".

These lectures were recorded and made available through the MARVEL website on slideshot.epfl.ch/events/14.

Internal communication

1 Review and Retreat

The third Review and Retreat took place at EPFL on Sep 7 and 8, 2016. This edition gathered 108 MARVEL participants (group leaders, senior researchers, postdocs and PhD students), representing 38 of the 40 research groups (Fig. 1). The Scientific Advisory Board was invited to attend the whole meeting. The program included 10 highlight talks covering MARVEL achievements by junior scientists. 3 moments were dedicated to the poster session — with standing lunch and during the photo exhibition (see 3.1) on the first day, and only with the junior scientists on the second day — to allow ample time around the 48 posters for discussing possible synergies and collaborations between the different projects (Fig. 1 right). Friday morning was devoted to individual project meetings: they elaborated their achievements for this report, set up action items for years 3 and 4, and planned/implemented collaborative papers. In parallel to the Friday poster session, all group leaders brainstormed on the phase 2 pre-proposal. This session included

Figure 1: *Third MARVEL Review and Retreat on Sep 7 – 8, 2016, at EPFL.*

short pitches presenting first ideas of potential research projects. The Scientific Advisory Board prepared a report presented to the director with comments and recommendations.

2 Other meetings

Since the last report, project meetings and other meetings of MARVEL groups took place regularly. These meetings are strongly encouraged by the NCCR direction, aiming at fostering collaboration and synergy between the different groups. As examples, PP7 experiments project had a meeting with all its participants on Mar 3, 2016 and a new meeting will take place on Apr 4, 2017 at PSI. The director also did one-on-one calls or meetings with all computational groups leaders throughout the summer and discussed with them the accomplishments of the project, their research and how to move forward. All computational group leaders and the three PP7 leaders met 3 times in Bern (Jul 21, Nov 4 and Dec 14, 2016) in order to collectively reflect on MARVEL's achievements, on the implementation of the structural measures, and on the second phase of the NCCR, to prepare the phase 2 pre-proposal.

3 MARVEL junior seminars

To intensify interactions between the MARVEL junior scientists based at EPFL, the MARVEL junior seminars were implemented and are taking place monthly since Nov 2016, with 30 – 40 participants, to initiate additional collaborations between research groups, and to establish a vibrant community. The organizing committee consists of 7 delegates among PhD students and postdocs representing EPFL research group and acting as chairperson. Each seminar includes two presentations on a scientific question explored in depth and followed by a discussion facilitated by the chairperson of the day (Fig. 2). The chairperson's mission is to ensure active lively interactions between the audience and the speakers. The program is communicated to the whole MARVEL community and to the associated EPFL research groups, and advertised on the website. Pizza is offered before the seminar, and coffee and pies after, to allow for scientific and informal discussion.

Figure 2: *MARVEL junior seminar at EPFL.*

External communication

1 Movies

The RTS Court du jour *Imaginez un monde. Les matériaux de demain*, shot in 2015, is also available in German, through the participation of ARTE (future.arte.tv/de/materialien-der-zukunft) and the English version is under development (available soon).
Two short 1-min movies, one in English (www.youtube.com/watch?v=5PiCNr_b_E) and one in French (www.youtube.com/watch?v=if6k3GmQctk), with Nicola Marzari presenting MARVEL, were shot by Alban Kakulya for the inauguration of the new ME D building upon request of the School of Engineering of EPFL.
These movies are to be used for communication purposes and available for various opportunities. They will be made visible through the website.

2 Events

2.1 Ig Nobel Award Tour Show

MARVEL sponsored and co-organized with EPFL the coming of the Ig Nobel Award Tour Show 2016 on Mar 23, 2016. At this occasion,

Figure 3: *Top: Ig Nobel Award Tour Show 2016 on Mar 23, 2016 at EPFL, poster and selected moments. Bottom: EPFL Open Days on Nov 5 – 6, 2016 with an interested public and fruitful discussions.*

the public could learn about "achievements that first make people laugh, and then make them think" as, e.g., the fact that "dung beetles use the Milky Way for navigation" (Fig. 3 top). The show will come again on Mar 21, 2017 with 3 new Ig Nobel laureates.

2.2 Inauguration of ME D building

The ME D building, in which MARVEL management and direction moved in Nov 2015, was inaugurated on May 10, 2016. The building was designed by the French architect Dominique Perrault and also hosts the NCCR Robotics. This was the opportunity to present MARVEL activities to the press and the public in the new distant education classroom "CoViz2" part of the EPFL commitment.

2.3 EPFL Open Days

EPFL organized general Open Days of the campus on Nov 5 – 6, 2016 with 35'000 visitors over the 2 days. MARVEL was present with 3D movies and some animations already proposed by the Marzari and Ceriotti groups at Scientastic in 2015. Two new 3D movies were developed for the occasion, one in the Pasquarello group and one in the Marzari group, as well as new animations. Besides the stereoscopic movies presented on a large screen, MARVEL showed a series of activities related to its research (Fig. 3 bottom). Over 30 people from 4 MARVEL groups (Ceriotti, Corminboeuf, Marzari, Pasquarello) were involved either in the preparation or in the animation of this event. A special thank to Mark Sawley from the "Application-Centered Computational Engineering Science" (ACCES) collaboration at EPFL without whose help no stereoscopic movies would have been displayed. The booth raised a sustained interest from a public of all ages and fruitful moments of exchanges with the researchers (Fig. 3 bottom).

3 Artistic work

3.1 Photography exhibition by Julie Birenbaum

The contacts initiated in 2014 by Nicola Spaldin with Julie Birenbaum, the light painting artist, resulted in a photography exhibition presented in the ME D hall at EPFL and inaugurated during the MARVEL Review and Retreat on Sep 8,

Figure 4: *Photography exhibition of Julie Birenbaum in the ME D hall at the MARVEL Review and Retreat, with Nicola Marzari and Julie Birenbaum.*

2016 in presence of the artist (Fig. 4). Initially planned for 2.5 weeks , it was prolonged to be present during the EPFL Open Days in Nov. As the space is available, the exhibition is still in place end of Jan 2017, bringing nice colors in the ME D hall. The exhibition is planned to be then presented at ETHZ.

3.2 Visualization contest

The next edition of the visualization contest at EPFL will take place in the second part of 2017.

4 Other communication-related actions

MARVEL participates in the monthly meeting of all EPFL communication officers to guarantee a good cooperation with the host institution partners.

5 MARVEL in web news and in the press

A feature story in *Nature* prominently presented MARVEL and interviewed Profs. Smit and Marzari [224]. MARVEL was mentioned several times in the electronic news of EPFL, with the promotion of hot research topics, and in the internal *Flash* and *EPFL Magazine* newspapers. Outside EPFL, some news in relationship with MARVEL were published on the websites of other MARVEL-involved institutions. For example, several press releases were made related to [136] in the von Lilienfeld group (tinyurl.com/hs2yne6). These news were usually relayed on the MARVEL website and will be included in the newsletter. They are also listed in the NIRA database.

9 Structural aspects

Most of the contractual structural measures have already been implemented during years 1 and 2, with the set-up of the visualization room "CoViz1" in MXC 320 and the storage hardware co-located at CSCS. In addition, extra measures, not in the initial commitment, included moving the headquarters of MARVEL to the new ME D building and creating the distant education classroom "CoViz2".

The promised tenure-track positions in computational materials science and condensed matter physics were allocated to Michele Ceriotti in Materials and to Oleg Yazyev in Physics. The third tenure-track assistant professor in the School of Computer and Communication Sciences was allocated to Martin Jaggi, who works in the field of machine learning and optimization, and who will be associated to MARVEL from May 2017 through an "Agility Plus" project. All the home institution's commitments were thus accomplished or improved upon.

MARVEL-related publications

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

[1] S. Keller, M. Dolfi, M. Troyer, and M. Reiher, *An efficient matrix product operator representation of the quantum chemical Hamiltonian*, The Journal of Chemical Physics **143**, 244118 (2015).

[2] A. A. Soluyanov, D. Gresch, Z. Wang, Q. Wu, M. Troyer, X. Dai, and B. A. Bernevig, *Type-II Weyl semimetals*, Nature **527**, 495 (2015).

[3] T. Bzdušek, Q. Wu, A. Rüegg, M. Sigrist, and A. A. Soluyanov, *Nodal-chain metals*, Nature **538**, 75 (2016).

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

[5] N. Xu, H. M. Weng, B. Q. Lv, C. E. Matt, J. Park, F. Bisti, V. N. Strocov, D. Gawryluk, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, G. Autès, O. V. Yazyev, Z. Fang, X. Dai, T. Qian, J. Mesot, H. Ding, and M. Shi, *Observation of Weyl nodes and Fermi arcs in tantalum phosphide*, Nature Communications **7**, 11006 (2016).

[6] G. Autès, D. Gresch, M. Troyer, A. A. Soluyanov, and O. V. Yazyev, *Robust Type-II Weyl Semimetal Phase in Transition Metal Diphosphides XP_2 (X = Mo, W)*, Physical Review Letters **117**, 066402 (2016).

[7] G. W. Winkler, Q. Wu, M. Troyer, P. Krogstrup, and A. A. Soluyanov, *Topological Phases in $InAs_{1-x}Sb_x$: From Novel Topological Semimetal to Majorana Wire*, Physical Review Letters **117**, 076403 (2016).

[8] G. Manzoni, L. Gragnaniello, G. Autès, T. Kuhn, A. Sterzi, F. Cilento, M. Zacchigna, V. Enenkel, I. Vobornik, L. Barba, F. Bisti, P. Bugnon, A. Magrez, V. N. Strocov, H. Berger, O. V. Yazyev, M. Fonin, F. Parmigiani, and A. Crepaldi, *Evidence for a Strong Topological Insulator Phase in $ZrTe_5$*, Physical Review Letters **117**, 237601 (2016).

[9] Z. Zhu, G. W. Winkler, Q. Wu, J. Li, and A. A. Soluyanov, *Triple Point Topological Metals*, Physical Review X **6**, 031003 (2016).

[10] A. Tamai, Q. S. Wu, I. Cucchi, F. Y. Bruno, S. Riccò, T. K. Kim, M. Hoesch, C. Barreteau, E. Giannini, C. Besnard, A. A. Soluyanov, and F. Baumberger, *Fermi Arcs and Their Topological Character in the Candidate Type-II Weyl Semimetal* $MoTe_2$, Physical Review X **6**, 031021 (2016).

[11] A. Subedi, O. E. Peil, and A. Georges, *Low-energy description of the metal-insulator transition in the rare-earth nickelates*, Physical Review B **91**, 075128 (2015).

[12] J. Ruppen, J. Teyssier, O. E. Peil, S. Catalano, M. Gibert, J. Mravlje, J.-M. Triscone, A. Georges, and D. van der Marel, *Optical spectroscopy and the nature of the insulating state of rare-earth nickelates*, Physical Review B **92**, 155145 (2015).

[13] M. Aichhorn, L. Pourovskii, P. Seth, V. Vildosola, M. Zingl, O. E. Peil, X. Deng, J. Mravlje, G. J. Kraberger, C. Martins, M. Ferrero, and O. Parcollet, *TRIQS/DFTTools: A TRIQS application for* ab initio *calculations of correlated materials*, Computer Physics Communications **204**, 200 (2016).

[14] G. Sclauzero and C. Ederer, *Structural and electronic properties of epitaxially strained $LaVO_3$ from density functional theory and dynamical mean-field theory*, Physical Review B **92**, 235112 (2015).

[15] G. Sclauzero, K. Dymkowski, and C. Ederer, *Tuning the metal-insulator transition in d^1 and d^2 perovskites by epitaxial strain: a first principles-based study*, Physical Review B **94**, 245109 (2016).

[16] M. Morin, A. Scaramucci, M. Bartkowiak, E. Pomjakushina, G. Deng, D. Sheptyakov, L. Keller, J. Rodriguez-Carvajal, N. A. Spaldin, M. Kenzelmann, K. Conder, and M. Medarde, *Incommensurate magnetic structure, Fe/Cu chemical disorder, and magnetic interactions in the high-temperature multiferroic $YBaCuFeO_5$*, Physical Review B **91**, 064408 (2015).

[17] 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*, arXiv:1610.00783 (2016).

[18] A. Scaramucci, H. Shinaoka, M. V. Mostovoy, M. Müller, and C. Mudry, *Spiral order from orientationally correlated random bonds in classical XY models*, arXiv:1610.00784 (2016).

[19] S. M. Griffin, P. Staar, T. C. Schulthess, M. Troyer, and N. A. Spaldin, *A bespoke single-band Hubbard model material*, Physical Review B **93**, 075115 (2016).

[20] D. Gresch, G. Autès, O. V. Yazyev, M. Troyer, D. Vanderbilt, B. A. Bernevig, and A. A. Soluyanov, *Z2Pack: Numerical Implementation of Hybrid Wannier Centers for Identifying Topological Materials*, arXiv:1610.08983, *to be published in* Physical Review B (2017), http://z2pack.ethz.ch.

[21] Z. Wang, D. Gresch, A. A. Soluyanov, W. Xie, S. Kushwaha, X. Dai, M. Troyer, R. J. Cava, and B. A. Bernevig, *$MoTe_2$: a type-II Weyl topological metal*, Physical Review Letters **117**, 056805 (2016).

[22] F. Y. Bruno, A. Tamai, Q. S. Wu, I. Cucchi, C. Barreteau, A. de la Torre, S. McKeown Walker, S. Riccò, Z. Wang, T. K. Kim, M. Hoesch, M. Shi, N. C. Plumb, E. Giannini, A. A. Soluyanov, and F. Baumberger, *Observation of large topologically trivial Fermi arcs in the candidate type-II Weyl semimetal* WTe_2, Physical Review B **94**, 121112 (2016).

[23] D. Gresch, Q. Wu, G. W. Winkler, and A. A. Soluyanov, *Hidden Weyl Points in Centrosymmetric Paramagnetic Metals*, arXiv:1611.01858 (2016).

[24] A. A. Soluyanov, D. Gresch, M. Troyer, R. M. Lutchyn, B. Bauer, and C. Nayak, *Optimizing spin-orbit splittings in InSb Majorana nanowires*, Physical Review B **93**, 115317 (2016).

[25] L. Tiemann, S. Mueller, Q. Wu, T. Tschirky, K. Ensslin, W. Wegscheider, M. Troyer, A. A. Soluyanov, and T. Ihn, *On the impact of strain on the electronic properties of InAs/GaSb quantum well systems*, arXiv:1610.06776 (2016).

[26] G. W. Winkler, A. A. Soluyanov, and M. Troyer, *Smooth gauge and Wannier functions for topological band structures in arbitrary dimensions*, Physical Review B **93**, 035453 (2016).

[27] G. Manzoni, A. Crepaldi, G. Autès, A. Sterzi, F. Cilento, A. Akrap, I. Vobornik, L. Gragnaniello, P. Bugnon, M. Fonin, H. Berger, M. Zacchigna, O. V. Yazyev, and F. Parmigiani, *Temperature dependent non-monotonic bands shift in $ZrTe_5$*, Journal of Electron Spectroscopy and Related Phenomena (2016), doi:10.1016/j.elspec.2016.09.006.

[28] S. Mathew, A. Yella, P. Gao, R. Humphry-Baker, B. F. E. Curchod, N. Ashari-Astani, I. Tavernelli, U. Rothlisberger, M. K. Nazeeruddin, and M. Grätzel, *Dye-sensitized solar cells with 13% efficiency achieved through the molecular engineering of porphyrin sensitizers*, Nature Chemistry **6**, 242 (2014).

- [29] K. Voïtchovsky, N. Ashari Astani, I. Tavernelli, N. Tétreault, U. Rothlisberger, F. Stellacci, M. Grätzel, and H. A. Harms, *In Situ Mapping of the Molecular Arrangement of Amphiphilic Dye Molecules at the TiO_2 Surface of Dye-Sensitized Solar Cells*, ACS Applied Materials & Interfaces **7**, 10834 (2015).
- [30] W. Tress, B. Beyer, N. Ashari Astani, F. Gao, S. Meloni, and U. Rothlisberger, *Extended Intermolecular Interactions Governing Photocurrent-Voltage Relations in Ternary Organic Solar Cells*, The Journal of Physical Chemistry Letters **7**, 3936 (2016).
- [31] C. Yi, J. Luo, S. Meloni, A. Boziki, N. Ashari-Astani, C. Grätzel, S. M. Zakeeruddin, U. Röthlisberger, and M. Grätzel, *Entropic stabilization of mixed A-cation ABX_3 metal halide perovskites for high performance perovskite solar cells*, Energy & Environmental Science **9**, 656 (2016).
- [32] S. Meloni, T. Moehl, W. Tress, M. Franckevičius, M. Saliba, Y. H. Lee, P. Gao, M. K. Nazeeruddin, S. M. Zakeeruddin, U. Rothlisberger, and M. Graetzel, *Ionic polarization-induced current-voltage hysteresis in $CH_3NH_3PbX_3$ perovskite solar cells*, Nature Communications **7**, 10334 (2016).
- [33] M. I. Dar, G. Jacopin, S. Meloni, A. Mattoni, N. Arora, A. Boziki, S. M. Zakeeruddin, U. Rothlisberger, and M. Grätzel, *Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites*, Science Advances **2**, e1601156 (2016).
- [34] S. Meloni, G. Palermo, N. Ashari-Astani, M. Grätzel, and U. Rothlisberger, *Valence and conduction band tuning in halide perovskites for solar cell applications*, Journal of Materials Chemistry A **4**, 15997 (2016).
- [35] A. Boziki, D. Tomerini, S. Goedecker, and U. Rothlisberger, *in preparation* (2016).
- [36] M. Busch, M. Wodrich, and C. Corminboeuf, *Linear Scaling Relationships and Volcano Plots in Homogeneous Catalysis ? Revisiting the Suzuki Reaction*, Chemical Science **6**, 6754 (2015).
- [37] M. Busch, M. Wodrich, and C. Corminboeuf, *A Generalized Picture of C-C Cross-Coupling, submitted* (2016).
- [38] M. Wodrich, M. Busch, and C. Corminboeuf, *Accessing and predicting the kinetic profiles of homogeneous catalysts from volcano plots*, Chemical Science **7**, 5723 (2016).
- [39] M. Schilling, G. R. Patzke, J. Hutter, and S. Luber, *Computational Investigation and Design of Cobalt Aqua Complexes for Homogeneous Water Oxidation*, The Journal of Physical Chemistry C **120**, 7966 (2016).
- [40] F. H. Hodel and S. Luber, *What Influences the Water Oxidation Activity of a Bioinspired Molecular $Co_4^{II}O_4$ Cubane? An In-Depth Exploration of Catalytic Pathways*, ACS Catalysis **6**, 1505 (2016).
- [41] F. H. Hodel and S. Luber, *Redox-Inert Cations Enhancing Water Oxidation Activity: The Crucial Role of Flexibility*, ACS Catalysis **6**, 6750 (2016).
- [42] G. Mette, D. Sutter, Y. Gurdal, S. Schnidrig, B. Probst, M. Iannuzzi, J. Hutter, R. Alberto, and J. Osterwalder, *From porphyrins to pyrphyrins: adsorption study and metalation of a molecular catalyst on Au(111)*, Nanoscale **8**, 7958 (2016).
- [43] Y. Gurdal, S. Luber, J. Hutter, and M. Iannuzzi, *Non-innocent adsorption of Co-pyrphyrin on rutile(110)*, Physical Chemistry Chemical Physics **17**, 22846 (2015).
- [44] F. Evangelisti, R. Moré, F. Hodel, S. Luber, and G. R. Patzke, *3d–4f $Co_3^{II}Ln(OR)_4$ Cubanes as Bio-Inspired Water Oxidation Catalysts*, Journal of the American Chemical Society **137**, 11076 (2015).
- [45] H. Liu, M. Schilling, M. Yulikov, S. Luber, and G. R. Patzke, *Homogeneous Photochemical Water Oxidation with Cobalt Chloride in Acidic Media*, ACS Catalysis **5**, 4994 (2015).
- [46] F. Song, M. Busch, B. Lassalle-Kaiser, E. Petkucheva, M. Bensimon, C. Corminboeuf, and X. Hu, *Bifunctional Catalysis for the Oxygen Evolution Reaction, submitted* (2016).
- [47] G. Miceli, S. de Gironcoli, and A. Pasquarello, *Isobaric first-principles molecular dynamics of liquid water with nonlocal van der Waals interactions*, The Journal of Chemical Physics **142**, 034501 (2015).
- [48] G. Miceli, J. Hutter, and A. Pasquarello, *Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets*, Journal of Chemical Theory and Computation **12**, 3456 (2016).
- [49] F. Ambrosio, G. Miceli, and A. Pasquarello, *Structural, dynamical, and electronic properties of liquid water: A hybrid functional study*, The Journal of Physical Chemistry B **120**, 7456 (2016).
- [50] F. Ambrosio, G. Miceli, and A. Pasquarello, *Redox levels in aqueous solution: Effect of van der Waals interactions and hybrid functionals*, The Journal of Chemical Physics **143**, 244508 (2015).
- [51] W. Chen and A. Pasquarello, *Band-edge positions in GW: Effects of starting point and self-consistency*, Physical Review B **90**, 165133 (2014).
- [52] W. Chen and A. Pasquarello, *Accurate band gaps of extended systems via efficient vertex corrections in GW*, Physical Review B **92**, 041115 (2015).
- [53] W. Chen and A. Pasquarello, *First-principles determination of defect energy levels through hybrid density functionals and GW*, Journal of Physics: Condensed Matter **27**, 133202 (2015).
- [54] W. Chen, F. Ambrosio, G. Miceli, and A. Pasquarello, *Ab initio electronic structure of liquid water*, Physical Review Letters **117**, 186401 (2016).
- [55] A. Marcolongo and N. Marzari, *Correlations boost conductivity in solid-state fast ion conductors, submitted* (2017).
- [56] A. Fluri, A. Marcolongo, V. Roddatis, A. Wokaun, D. Pergolesi, N. Marzari, and T. Lippert, *Enhanced Proton Conductivity in Y-doped $BaZrO_3$ via Strain Engineering, submitted* (2017).
- [57] T. Laino and V. Weber, *Sodium oxoferrate based ionic conductors* (2016), *Patent*.
- [58] K. Meier, T. Laino, and A. Curioni, *Solid-State Electrolytes: Revealing the Machanisms of Li-Ion Conduction in Tetragonal and Cubic LLZO by First-Principles Calculations*, The Journal of Physical Chemistry C **118**, 6668 (2014).
- [59] G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, and B. Kozinsky, *AiiDA: automated interactive infrastructure and database for computational science*, Computational Materials Science **111**, 218 (2016).
- [60] N. Mounet, M. Gibertini, P. Schwaller, A. Merkys, I. E. Castelli, A. Cepellotti, G. Pizzi, and N. Marzari, *Novel two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds*, arXiv:1611.05234 (2016).
- [61] H. Söde, L. Talirz, O. Gröning, C. A. Pignedoli, R. Berger, X. Feng, K. Müllen, R. Fasel, and P. Ruffieux, *Electronic band dispersion of graphene nanoribbons via Fourier-transformed scanning tunneling spectroscopy*, Physical Review B **91**, 045429 (2015).
- [62] S. Wang, L. Talirz, C. A. Pignedoli, X. Feng, K. Müllen, R. Fasel, and P. Ruffieux, *Giant edge state splitting at atomically precise graphene zigzag edges*, Nature Communications **7**, 11507 (2016).

[63] P. Ruffieux, S. Wang, B. Yang, C. Sánchez-Sánchez, J. Liu, T. Dienel, L. Talirz, P. Shinde, C. A. Pignedoli, D. Passerone, T. Dumslaff, X. Feng, K. Müllen, and R. Fasel, *On-surface synthesis of graphene nanoribbons with zigzag edge topology*, Nature **531**, 489 (2016).

[64] J. Cai, C. A. Pignedoli, L. Talirz, P. Ruffieux, H. Söde, L. Liang, V. Meunier, R. Berger, R. Li, X. Feng, K. Müllen, and R. Fasel, *Graphene nanoribbon heterojunctions*, Nature Nanotechnology **9**, 896 (2014).

[65] R. Denk, M. Hohage, P. Zeppenfeld, J. Cai, C. A. Pignedoli, H. Söde, R. Fasel, X. Feng, K. Müllen, S. Wang, D. Prezzi, A. Ferretti, A. Ruini, E. Molinari, and P. Ruffieux, *Exciton-dominated optical response of ultra-narrow graphene nanoribbons*, Nature Communications **5**, 4253 (2014).

[66] R. Jaafar, C. A. Pignedoli, G. Bussi, K. Aït-Mansour, O. Groening, T. Amaya, T. Hirao, R. Fasel, and P. Ruffieux, *Bowl Inversion of Surface-Adsorbed Sumanene*, Journal of the American Chemical Society **136**, 13666 (2014).

[67] S. Kawai, A. Benassi, E. Gnecco, H. Söde, R. Pawlak, X. Feng, K. Müllen, D. Passerone, C. A. Pignedoli, P. Ruffieux, R. Fasel, and E. Meyer, *Superlubricity of graphene nanoribbons on gold surfaces*, Science **351**, 957 (2016).

[68] G. Fugallo, A. Cepellotti, L. Paulatto, M. Lazzeri, N. Marzari, and F. Mauri, *Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths*, Nano Letters **14**, 6109 (2014).

[69] A. Cepellotti, G. Fugallo, L. Paulatto, M. Lazzeri, F. Mauri, and N. Marzari, *Phonon hydrodynamics in two-dimensional materials*, Nature Communications **6**, 6400 (2015).

[70] A. Cepellotti and N. Marzari, *Thermal Transport in Crystals as a Kinetic Theory of Relaxons*, Physical Review X **6**, 041013 (2016).

[71] M. Gibertini, G. Pizzi, and N. Marzari, *Engineering polar discontinuities in honeycomb lattices*, Nature Communications **5**, 5157 (2014).

[72] M. Gibertini and N. Marzari, *Emergence of One-Dimensional Wires of Free Carriers in Transition-Metal-Dichalcogenide Nanostructures*, Nano Letters **15**, 6229 (2015).

[73] G. Pizzi, M. Gibertini, E. Dib, N. Marzari, G. Iannaccone, and G. Fiori, *Performance of arsenene and antimonene double-gate MOSFETs from first principles*, Nature Communications **7**, 12585 (2016).

[74] C. Ma, F. Pietrucci, and W. Andreoni, *Reaction dynamics of CO_2 in aqueous amines from ab initio molecular dynamics: 2-amino-2-methyl-1,3-propanediol (AMPD) compared to monoethanolamine (MEA)*, Theoretical Chemistry Accounts **135**, 60 (2016).

[75] W. Andreoni and F. Pietrucci, *CO_2 capture in amine solutions: modelling and simulations with non-empirical methods*, Journal of Physics: Condensed Matter **28**, 503003 (2016).

[76] M. Iazzi and M. Troyer, *Efficient continuous-time quantum Monte Carlo algorithm for fermionic lattice models*, Physical Review B **91**, 241118 (2015).

[77] L. Wang, M. Iazzi, P. Corboz, and M. Troyer, *Efficient continuous-time quantum Monte Carlo method for the ground state of correlated fermions*, Physical Review B **91**, 235151 (2015).

[78] H. Shinaoka, Y. Nomura, S. Biermann, M. Troyer, and P. Werner, *Negative sign problem in continuous-time quantum Monte Carlo: optimal choice of single-particle basis for impurity problems*, Physical Review B **92**, 195126 (2015).

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

[80] G. Borghi, A. Ferretti, N. L. Nguyen, I. Dabo, and N. Marzari, *Koopmans-compliant functionals and their performance against reference molecular data*, Physical Review B **90**, 075135 (2014).

[81] A. Ferretti, I. Dabo, M. Cococcioni, and N. Marzari, *Bridging density-functional and many-body perturbation theory: Orbital-density dependence in electronic-structure functionals*, Physical Review B **89**, 195134 (2014).

[82] N. L. Nguyen, G. Borghi, A. Ferretti, and N. Marzari, *First-Principles Photoemission Spectroscopy of DNA and RNA Nucleobases from Koopmans-Compliant Functionals*, Journal of Chemical Theory and Computation **12**, 3948 (2016).

[83] V. V. Rybkin and J. VandeVondele, *Spin-Unrestricted Second-Order Møller-Plesset (MP2) Forces for the Condensed Phase: From Molecular Radicals to F-Centers in Solids*, Journal of Chemical Theory and Computation **12**, 2214 (2016).

[84] M. Del Ben, O. Schütt, T. Wentz, P. Messmer, J. Hutter, and J. VandeVondele, *Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution*, Computer Physics Communications **187**, 120 (2015).

[85] J. Wilhelm, P. Seewald, M. Del Ben, and J. Hutter, *Large-Scale Cubic-Scaling Random Phase Approximation Correlation Energy Calculations Using a Gaussian Basis*, Journal of Chemical Theory and Computation **12**, 5851 (2016).

[86] J. Wilhelm, M. Del Ben, and J. Hutter, *GW in the Gaussian and Plane Waves Scheme with Application to Linear Acenes*, Journal of Chemical Theory and Computation **12**, 3623 (2016).

[87] M. Del Ben, J. Hutter, and J. VandeVondele, *Probing the structural and dynamical properties of liquid water with models including non-local electron correlation*, The Journal of Chemical Physics **143**, 054506 (2015).

[88] M. Del Ben, J. Hutter, and J. VandeVondele, *Forces and stress in second order Møller-Plesset perturbation theory for condensed phase systems within the resolution-of-identity Gaussian and plane waves approach*, The Journal of Chemical Physics **143**, 102803 (2015).

[89] J. Cheng and J. VandeVondele, *Calculation of Electrochemical Energy Levels in Water Using the Random Phase Approximation and a Double Hybrid Functional*, Physical Review Letters **116**, 086402 (2016).

[90] I. Timrov, O. Andreussi, A. Biancardi, N. Marzari, and S. Baroni, *Self-consistent continuum solvation for optical absorption of complex molecular systems in solution*, The Journal of Chemical Physics **142**, 034111 (2015).

[91] O. Andreussi and N. Marzari, *Electrostatics of solvated systems in periodic boundary conditions*, Physical Review B **90**, 245101 (2014).

[92] G. Fisicaro, L. Genovese, O. Andreussi, N. Marzari, and S. Goedecker, *A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments*, The Journal of Chemical Physics **144**, 014103 (2016).

[93] L. Wang, Y.-H. Liu, M. Iazzi, M. Troyer, and G. Harcos, *Split Orthogonal Group: A Guiding Principle for Sign-Problem-Free Fermionic Simulations*, Physical Review Letters **115**, 250601 (2015).

[94] Y.-H. Liu and L. Wang, *Quantum Monte Carlo study of mass-imbalanced Hubbard models*, Physical Review B **92**, 235129 (2015).

[95] L. Wang, Y.-H. Liu, J. Imriška, P. N. Ma, and M. Troyer, *Fidelity Susceptibility Made Simple: A Unified Quantum Monte Carlo Approach*, Physical Review X **5**, 031007 (2015).

[96] L. Wang, H. Shinaoka, and M. Troyer, *Fidelity Susceptibility Perspective on the Kondo Effect and Impurity Quantum Phase Transitions*, Physical Review Letters **115**, 236601 (2015).

[97] H. Shinaoka, M. Troyer, and P. Werner, *Accuracy of downfolding based on the constrained random-phase approximation*, Physical Review B **91**, 245156 (2015).

[98] L. Huang, T. Ayral, S. Biermann, and P. Werner, *Extended dynamical mean-field study of the Hubbard model with long-range interactions*, Physical Review B **90**, 195114 (2014).

[99] V. Kapil, J. VandeVondele, and M. Ceriotti, *Accurate molecular dynamics and nuclear quantum effects at low cost by multiple steps in real and imaginary time: Using density functional theory to accelerate wavefunction methods*, The Journal of Chemical Physics **144**, 054111 (2016).

[100] G. Fisicaro, L. Genovese, O. Andreussi, S. Mandal, N. N. Nair, N. Marzari, and S. Goedecker, *Soft-sphere continuum solvation in electronic-structure calculations*, *submitted* (2016).

[101] O. Valsson and M. Parrinello, *Variational Approach to Enhanced Sampling and Free Energy Calculations*, Physical Review Letters **113**, 090601 (2014).

[102] C. Perego, M. Salvalaglio, and M. Parrinello, *Molecular dynamics simulations of solutions at constant chemical potential*, The Journal of Chemical Physics **142**, 144113 (2015).

[103] M. Salvalaglio, C. Perego, F. Giberti, M. Mazzotti, and M. Parrinello, *Molecular-dynamics simulations of urea nucleation from aqueous solution*, Proceedings of the National Academy of Science of the USA **112**, E6 (2015).

[104] M. Salvalaglio, M. Mazzotti, and M. Parrinello, *Urea homogeneous nucleation mechanism is solvent dependent*, Faraday Discussions (2015), doi:10.1039/C4FD00235K.

[105] N. J. Browning, R. Ramakrishnan, O. A. von Lilienfeld, and U. Röthlisberger, *Genetic optimization of training sets for improved machine learning models of molecular properties*, arXiv:1611.07435 (2016).

[106] B. Schaefer, S. Mohr, M. Amsler, and S. Goedecker, *Minima hopping guided path search: An efficient method for finding complex chemical reaction pathways*, The Journal of Chemical Physics **140**, 214102 (2014).

[107] B. Schaefer, S. A. Ghasemi, S. Roy, and S. Goedecker, *Stabilized quasi-Newton optimization of noisy potential energy surfaces*, The Journal of Chemical Physics **142**, 034112 (2015).

[108] B. Schaefer and S. Goedecker, *Computationally efficient characterization of potential energy surfaces based on fingerprint distances*, The Journal of Chemical Physics **145**, 034101 (2016).

[109] L. Zhu, M. Amsler, T. Fuhrer, B. Schaefer, S. Faraji, S. Rostami, S. A. Ghasemi, A. Sadeghi, M. Grauzinyte, C. Wolverton, and S. Goedecker, *A fingerprint based metric for measuring similarities of crystalline structures*, The Journal of Chemical Physics **144**, 034203 (2016).

[110] O. Valsson and M. Parrinello, *Well-Tempered Variational Approach to Enhanced Sampling*, Journal of Chemical Theory and Computation **11**, 1996 (2015).

[111] P. Shaffer, O. Valsson, and M. Parrinello, *Enhanced, targeted sampling of high-dimensional free-energy landscapes using variationally enhanced sampling, with an application to chignolin*, Proceedings of the National Academy of Science of the USA **113**, 1150 (2016).

[112] J. McCarty, O. Valsson, P. Tiwary, and M. Parrinello, *Variationally Optimized Free-Energy Flooding for Rate Calculation*, Physical Review Letters **115**, 070601 (2015).

[113] J. McCarty, O. Valsson, and M. Parrinello, *Bespoke Bias for Obtaining Free Energy Differences within Variationally Enhanced Sampling*, Journal of Chemical Theory and Computation **12**, 2162 (2016).

[114] P. M. Piaggi, O. Valsson, and M. Parrinello, *A variational approach to nucleation simulation*, Faraday Discussions **195**, 557 (2016).

[115] M. Invernizzi, O. Valsson, and M. Parrinello, *Coarse graining from variationally enhanced sampling: The case of Ginzburg-Landau model*, *submitted* (2016).

[116] M. Salvalaglio, P. Tiwary, G. M. Maggioni, M. Mazzotti, and M. Parrinello, *Overcoming time scale and finite size limitations to compute nucleation rates from small scale well tempered metadynamics simulations*, The Journal of Chemical Physics **145**, 211925 (2016).

[117] C. Perego, F. Giberti, and M. Parrinello, *Chemical potential calculations in dense liquids using metadynamics*, The European Physical Journal – Special Topics **225**, 1621 (2016).

[118] A. Ozcan, C. Perego, M. Salvalaglio, M. Parrinello, and O. Yazaydin, *Concentration gradient driven molecular dynamics: A new method for simulations of membrane permeation and separation*, *submitted* (2016).

[119] J. A. Flores-Livas, M. Amsler, C. Heil, A. Sanna, L. Boeri, G. Profeta, C. Wolverton, S. Goedecker, and E. K. U. Gross, *Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure*, Physical Review B **93**, 020508 (2016).

[120] M. Amsler, S. Botti, M. A. L. Marques, T. J. Lenosky, and S. Goedecker, *Low-density silicon allotropes for photovoltaic applications*, Physical Review B **92**, 014101 (2015).

[121] K. Lejaeghere, G. Bihlmayer, T. Björkman, P. Blaha, S. Blügel, V. Blum, D. Caliste, I. E. Castelli, S. J. Clark, A. Dal Corso, S. de Gironcoli, T. Deutsch, J. K. Dewhurst, I. Di Marco, C. Draxl, M. Dulak, O. Eriksson, J. A. Flores-Livas, K. F. Garrity, L. Genovese, P. Giannozzi, M. Giantomassi, S. Goedecker, X. Gonze, O. Grånäs, E. K. U. Gross, A. Gulans, F. Gygi, D. R. Hamann, P. J. Hasnip, N. A. W. Holzwarth, D. Iuşan, D. B. Jochym, F. Jollet, D. Jones, G. Kresse, K. Koepernik, E. Küçükbenli, Y. O. Kvashnin, I. L. M. Locht, S. Lubeck, M. Marsman, N. Marzari, U. Nitzsche, L. Nordström, T. Ozaki, L. Paulatto, C. J. Pickard, W. Poelmans, M. I. J. Probert, K. Refson, M. Richter, G.-M. Rignanese, S. Saha, M. Scheffler, M. Schlipf, K. Schwarz, S. Sharma, F. Tavazza, P. Thunström, A. Tkatchenko, M. Torrent, D. Vanderbilt, M. J. van Setten, V. Van Speybroeck, J. M. Wills, J. R. Yates, G.-X. Zhang, and S. Cottenier, *Reproducibility in density functional theory calculations of solids*, Science **351**, 6280 (2016).

[122] P. Gasparotto and M. Ceriotti, *Recognizing molecular patterns by machine learning: An agnostic structural definition of the hydrogen bond*, The Journal of Chemical Physics **141**, 174110 (2014).

[123] S. De, A. P. Bartók, G. Csányi, and M. Ceriotti, *Comparing molecules and solids across structural and alchemical space*, Physical Chemistry Chemical Physics **18**, 13754 (2016).

[124] S. De, F. Musil, T. Ingram, C. Baldauf, and M. Ceriotti, *Mapping and classifying molecules from a high-throughput structural database*, Journal of Cheminformatics **9**, 6 (2017).

[125] P. Gasparotto, A. A. Hassanali, and M. Ceriotti, *Probing Defects and Correlations in the Hydrogen-Bond Network of ab Initio Water*, Journal of Chemical Theory and Computation **12**, 1953 (2016).

[126] R. Petraglia, A. Nicolaï, M. D. Wodrich, M. Ceriotti, and C. Corminboeuf, *Beyond Static Structures: Putting Forth REMD as a Tool to Solve Problems in Computational Organic Chemistry*, Journal of Computational Chemistry **37**, 83 (2016).

[127] M. Rossi, P. Gasparotto, and M. Ceriotti, *Anharmonic and Quantum Fluctuations in Molecular Crystals: A First-Principles Study of the Stability of Paracetamol*, Physical Review Letters **117**, 115702 (2016).

[128] G. Cuendet, A.-N. Ciubotaru, P. Staar, C. Bekas, and M. Gabrani, *TRADUCE meets LISIBLE: Automatic data extraction from scientific figures*, *submitted* (2017).

[129] P. Staar, M. Mottet, R. Istrate, M. Gabrani, and C. Bekas, *Technical document understanding with the SmartAnnotator tool: a teachable pipeline for documents in pdf-format*, *submitted* (2017).

[130] P. W. J. Staar, P. K. Barkoutsos, R. Istrate, A. C. I. Malossi, I. Tavernelli, N. Moll, H. Giefers, C. Hagleitner, C. Bekas, and A. Curioni, *Stochastic matrix-function estimators: Scalable Big-Data kernels with high performance*, in *2016 IEEE International Parallel and Distributed Processing Symposium (IPDPS)* (2016), p. 812, doi:10.1109/IPDPS.2016.34.

[131] R. Ramakrishnan, P. O. Dral, M. Rupp, and O. A. von Lilienfeld, *Big Data Meets Quantum Chemistry Approximations: The Δ-Machine Learning Approach*, Journal of Chemical Theory and Computation **11**, 2087 (2015).

[132] T. Bereau, D. Andrienko, and O. A. von Lilienfeld, *Transferable atomic multipole machine learning models for small organic molecules*, Journal of Chemical Theory and Computation **11**, 3225 (2015).

[133] M. Rupp, R. Ramakrishnan, and O. A. von Lilienfeld, *Machine Learning for Quantum Mechanical Properties of Atoms in Molecules*, The Journal of Physical Chemistry Letters **6**, 3309 (2015).

[134] R. Ramakrishnan, M. Hartmann, E. Tapavicza, and O. A. von Lilienfeld, *Electronic Spectra from TDDFT and Machine Learning in Chemical Space*, The Journal of Chemical Physics **143**, 084111 (2015).

[135] F. Faber, A. Lindmaa, O. A. von Lilienfeld, and R. Armiento, *Crystal Structure Representations for Machine Learning Models of Formation Energies*, International Journal of Quantum Chemistry **115**, 1094 (2015).

[136] F. A. Faber, A. Lindmaa, O. A. von Lilienfeld, and R. Armiento, *Machine Learning Energies of 2 Million Elpasolite (ABC_2D_6) Crystals*, Physical Review Letters **117**, 135502 (2016).

[137] B. Huang and O. A. von Lilienfeld, *Understanding molecular representations in machine learning: The role of uniqueness and target similarity*, The Journal of Chemical Physics **145**, 161102 (2016).

[138] A. Solovyeva and O. A. von Lilienfeld, *Alchemical Screening of Ionic Crystals*, Physical Chemistry Chemical Physics **18**, 31078 (2016).

[139] M. to Baben, J. O. Achenbach, and O. A. von Lilienfeld, *Guiding* ab initio *calculations by alchemical derivatives*, The Journal of Chemical Physics **144**, 104103 (2016).

[140] K. Y. S. Chang, S. Fias, R. Ramakrishnan, and O. A. von Lilienfeld, *Fast and accurate predictions of covalent bonds in chemical space*, The Journal of Chemical Physics **144**, 174110 (2016).

[141] D. E. Carlson, E. Collins, Y.-P. Hsieh, L. Carin, and V. Cevher, *Preconditioned Spectral Descent for Deep Learning*, in *Advances in Neural Information Processing Systems 28 (NIPS 2015)*, C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, eds. (2015).

[142] A. Norouzi-Fard, A. Bazzi, I. Bogunovic, M. El Halabi, Y.-P. Hsieh, and V. Cevher, *An Efficient Streaming Algorithm for the Submodular Cover Problem*, in *Advances in Neural Information Processing Systems 29 (NIPS 2016)*, D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett., eds. (2016).

[143] *Domain specific library for electronic structure calculations*, https://github.com/electronic-structure/SIRIUS.

[144] T. C. Schulthess, *Programming revisited*, Nature Physics **11**, 369 (2015).

[145] Y. Hinuma, G. Pizzi, Y. Kumagai, F. Oba, and I. Tanaka, *Band structure diagram paths based on crystallography*, Computational Materials Science **128**, 140 (2017).

[146] R. Solcà, A. Kozhevnikov, A. Haidar, S. Tomov, J. Dongarra, and T. C. Schulthess, *Efficient implementation of quantum materials simulations on distributed CPU-GPU systems*, in *SC'15, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis* (ACM, New York, 2015), article No. 10, doi:10.1145/2807591.2807654.

[147] X. Cheng, E. Fabbri, M. Nachtegaal, I. E. Castelli, M. El Kazzi, R. Haumont, N. Marzari, and T. J. Schmidt, *Oxygen Evolution Reaction on $La_{1-x}Sr_xCoO_3$ Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties*, Chemistry of Materials **27**, 7662 (2015).

[148] N. Xu, H. Ding, and M. Shi, *Spin- and angle-resolved photoemission on the topological Kondo insulator candidate: SmB_6*, Journal of Physics: Condensed Matter **28**, 363001 (2016).

[149] F. Evangelisti, M. Stiefel, O. Guseva, R. P. Nia, R. Hauert, E. Hack, L. P. H. Jeurgens, F. Ambrosio, A. Pasquarello, P. Schmutz, and C. Cancellieri, *Electronic and structural characterization of barrier-type amorphous aluminium oxide*, Electrochimica Acta **224**, 503 (2017).

[150] F. Evangelisti, R. Güttinger, R. Moré, S. Luber, and G. R. Patzke, *Closer to Photosystem II: A Co_4O_4 Cubane Catalyst with Flexible Ligand Architecture*, Journal of the American Chemical Society **135**, 18734 (2013).

[151] E. Gilardi, E. Fabbri, L. Bi, J. L. M. Rupp, A. Wokaun, T. Lippert, D. Pergolesi, and E. Traversa, *Effect of dopant — host ionic radii mismatch on acceptor doped barium zirconate microstructure and proton conductivity*, *submitted* (2016).

Other references

[152] K. Dymkowski and C. Ederer, *Strain-induced insulator-to-metal transition in $LaTiO_3$ within DFT+DMFT*, Physical Review B **89**, 161109 (2014).

[153] C. He, T. D. Sanders, M. T. Gray, F. J. Wong, V. V. Mehta, and Y. Suzuki, *Metal-insulator transitions in epitaxial $LaVO_3$ and $LaTiO_3$ films*, Physical Review B **86**, 081401 (2012).

[154] M. Morin, E. Canévet, A. Raynaud, M. Bartkowiak, D. Sheptyakov, V. Ban, M. Kenzelmann, E. Pomjakushina, K. Conder, and M. Medarde, *Tuning magnetic spirals beyond room temperature with chemical disorder*, arXiv:1608.03372 (2016).

[155] S. Artyukhin, K. T. Delaney, N. A. Spaldin, and M. Mostovoy, *Landau theory of topological defects in multiferroic hexagonal manganites*, Nature Materials **13**, 42 (2014).

[156] R. M. Lutchyn, J. D. Sau, and S. D. Sarma, *Majorana fermions and a topological phase transition in semiconductor-superconductor heterostructures*, Physical Review Letters **105**, 077001 (2010).

[157] Y. Oreg, G. Refael, and F. von Oppen, *Helical liquids and Majorana bound states in quantum wires*, Physical Review Letters **105**, 177002 (2010).

[158] S. Das Sarma, M. Freedman, and C. Nayak, *Topological quantum computation*, Physics Today **59**, 32 (2006).

[159] C. L. Kane and E. J. Mele, *Z_2 topological order and the quantum spin Hall effect*, Physical Review Letters **95**, 146802 (2005).

[160] A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt, and N. Marzari, *wannier90: A tool for obtaining maximally-localised Wannier functions.*, Computer Physics Communications **178**, 685 (2008).

[161] C. C. Stoumpos, C. D. Malliakas, and M. G. Kanatzidis, *Semiconducting tin and lead iodide perovskites with organic cations: phase transitions, high mobilities, and near-infrared photoluminescent properties*, Inorganic Chemistry **52**, 9019 (2013).

[162] S. Goedecker, *Minima hopping: An efficient search method for the global minimum of the potential energy surface of complex molecular systems*, The Journal of Chemical Physics **120**, 9911 (2004).

[163] A. Mattoni, A. Filippetti, M. I. Saba, and P. Delugas, *Methylammonium Rotational Dynamics in Lead Halide Perovskite by Classical Molecular Dynamics: The Role of Temperature*, The Journal of Physical Chemistry C **119**, 17421 (2015).

[164] F. Evangelisti, R. Güttinger, R. Moré, S. Luber, and G. R. Patzke, *Closer to Photosystem II: A Co_4O_4 Cubane Catalyst with Flexible Ligand Architecture*, Journal of the American Chemical Society **135**, 18734 (2013).

[165] P. G. Balakrishnan, R. Ramesh, and T. Prem Kumar, *Safety mechanisms in lithium-ion batteries*, Journal of Power Sources **155**, 401 (2006).

[166] Y. Wang, W. D. Richards, S. P. Ong, L. J. Miara, J. C. Kim, Y. Mo, and G. Ceder, *Design principles for solid-state lithium superionic conductors*, Nature Materials **14**, 1026 (2015).

[167] N. Kamaya, K. Homma, Y. Yamakawa, M. Hirayama, R. Kanno, M. Yonemura, T. Kamiyama, Y. Kato, S. Hama, K. Kawamoto, and A. Mitsui, *A lithium superionic conductor*, Nature Materials **10**, 682 (2011).

[168] M. Klenk and W. Lai, *Local structure and dynamics of lithium garnet ionic conductors: tetragonal and cubic $Li_7La_3Zr_2O_7$*, Physical Chemistry Chemical Physics **17**, 8758 (2015).

[169] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, *Quantum ESPRESSO: a modular and open-source software project for quantum simulations of materials*, Journal of Physics: Condensed Matter **21**, 395502 (2009).

[170] C. H. Rycroft, *VORO++: A three-dimensional Voronoi cell library in C++*, Chaos: An Interdisciplinary Journal of Nonlinear Science **19**, 041111 (2009).

[171] http://www.fiz-karlsruhe.com/icsd.html.

[172] S. Gražulis, A. Daškevič, A. Merkys, D. Chateigner, L. Lutterotti, M. Quirós, N. R. Serebryanaya, P. Moeck, R. T. Downs, and A. Le Bail, *Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration*, Nucleic Acids Research **40**, D420 (2012).

[173] R. Sabatini, T. Gorni, and S. de Gironcoli, *Nonlocal van der Waals density functional made simple and efficient*, Physical Review B **87**, 041108 (2013).

[174] I. Hamada and M. Otani, *Comparative van der Waals density-functional study of graphene on metal surfaces*, Physical Review B **82**, 153412 (2010).

[175] P. Ruffieux, J. Cai, N. C. Plumb, L. Patthey, D. Prezzi, A. Ferretti, E. Molinari, X. Feng, K. Müllen, C. A. Pignedoli, and R. Fasel, *Electronic structure of atomically precise graphene nanoribbons*, ACS Nano **6**, 6930 (2012).

[176] C. A. Guido, F. Pietrucci, G. A. Gallet, and W. Andreoni, *The Fate of a Zwitterion in Water from* ab Initio *Molecular Dynamics: Monoethanolamine (MEA)-CO_2*, Journal of Chemical Theory and Computation **9**, 28 (2013).

[177] C. Ma, F. Pietrucci, and W. Andreoni, *Capturing CO_2 in Monoethanolamine (MEA) Aqueous Solutions: Fingerprints of Carbamate Formation Assessed with First-Principles Simulations*, The Journal of Physical Chemistry Letters **5**, 1672 (2014).

[178] C. Ma, F. Pietrucci, and W. Andreoni, *Capture and Release of CO_2 in Monoethanolamine Aqueous Solutions: New Insights from First-Principles Reaction Dynamics*, Journal of Chemical Theory and Computation **11**, 3189 (2015).

[179] E. Pavarini, S. Biermann, A. Poteryaev, A. I. Lichtenstein, A. Georges, and O. K. Andersen, *Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites*, Physical Review Letters **92**, 176403 (2004).

[180] I. A. Nekrasov, K. Held, G. Keller, D. E. Kondakov, T. Pruschke, M. Kollar, O. K. Andersen, V. I. Anisimov, and D. Vollhardt, *Momentum-resolved spectral functions of $SrVO_3$ calculated by* LDA + DMFT, Physical Review B **73**, 155112 (2006).

[181] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M. Cococcioni, *Koopmans' condition for density-functional theory*, Physical Review B **82**, 115121 (2010).

[182] T. A. Pham, C. Zhang, E. Schwegler, and G. Galli, *Probing the electronic structure of liquid water with many-body perturbation theory*, Physical Review B **89**, 060202 (2014).

[183] O. Andreussi, I. Dabo, and N. Marzari, *Revised self-consistent continuum solvation in electronic-structure calculations*, The Journal of Chemical Physics **136**, 064102 (2012).

[184] E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, *Continuous-time Monte Carlo methods for quantum impurity models*, Reviews of Modern Physics **83**, 349 (2011).

[185] S. Biermann, F. Aryasetiawan, and A. Georges, *First-Principles Approach to the Electronic Structure of*

Strongly Correlated Systems: Combining the GW Approximation and Dynamical Mean-Field Theory, Physical Review Letters **90**, 086402 (2003).

[186] T. Ayral, S. Biermann, and P. Werner, *Screening and nonlocal correlations in the extended Hubbard model from self-consistent combined GW and dynamical mean field theory*, Physical Review B **87**, 125149 (2013).

[187] P. Hansmann, T. Ayral, L. Vaugier, P. Werner, and S. Biermann, *Long-Range Coulomb Interactions in Surface Systems: A First-Principles Description within Self-Consistently Combined GW and Dynamical Mean-Field Theory*, Physical Review Letters **110**, 166401 (2013).

[188] H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner, *Nonequilibrium dynamical mean-field theory and its applications*, Reviews of Modern Physics **86**, 779 (2014).

[189] M. Guidon, J. Hutter, and J. VandeVondele, *Auxiliary Density Matrix Methods for Hartree-Fock Exchange Calculations*, Journal of Chemical Theory and Computation **6**, 2348 (2010).

[190] M. Del Ben, J. Hutter, and J. VandeVondele, *Electron Correlation in the Condensed Phase from a Resolution of Identity Approach Based on the Gaussian and Plane Waves Scheme*, Journal of Chemical Theory and Computation **9**, 2654 (2013).

[191] U. Borštnik, J. VandeVondele, V. Weber, and J. Hutter, *Sparse matrix multiplication: The distributed block-compressed sparse row library*, Parallel Computing **40**, 47 (2014).

[192] L.-C. Lin, A. H. Berger, R. L. Martin, J. Kim, J. A. Swisher, K. Jariwala, C. H. Rycroft, A. S. Bhown, M. W. Deem, M. Haranczyk, and B. Smit, In silico *screening of carbon-capture materials*, Nature Materials **11**, 633 (2012).

[193] C. M. Simon, J. Kim, L.-C. Lin, R. L. Martin, M. Haranczyk, and B. Smit, *Optimizing nanoporous materials for gas storage*, Physical Chemistry Chemical Physics **16**, 5499 (2014).

[194] S. K. Bhatia and A. L. Myers, *Optimum conditions for adsorptive storage*, Langmuir **22**, 1688 (2006).

[195] M. Amsler and S. Goedecker, *Crystal structure prediction using the minima hopping method*, The Journal of Chemical Physics **133**, 224104 (2010).

[196] S. Roy, S. Goedecker, and V. Hellmann, *Bell-Evans-Polanyi principle for molecular dynamics trajectories and its implications for global optimization*, Physical Review E **77**, 056707 (2008).

[197] M. Vejdemo-Johansson, *Sketches of a platypus: A survey of persistent homology and its algebraic foundations*, arXiv:1212.5398 (2013).

[198] G. A. Tribello, M. Bonomi, D. Branduardi, C. Camilloni, and G. Bussi, *PLUMED 2: New feathers for an old bird*, Computer Physics Communications **185**, 604 (2014).

[199] N. Pellet, P. Gao, G. Gregori, T.-Y. Yang, M. K. Nazeeruddin, J. Maier, and M. Grätzel, *Mixed-Organic-Cation Perovskite Photovoltaics for Enhanced Solar-Light Harvesting*, Angewandte Chemie International Edition **53**, 3151 (2014).

[200] N. J. Jeon, J. H. Noh, W. S. Yang, Y. C. Kim, S. Ryu, J. Seo, and S. I. Seok, *Compositional engineering of perovskite materials for high-performance solar cells*, Nature **517**, 476 (2015).

[201] M. Ceriotti, G. A. Tribello, and M. Parrinello, *From the Cover: Simplifying the representation of complex free-energy landscapes using sketch-map*, Proceedings of the National Academy of Science of the USA **108**, 13023 (2011).

[202] G. A. Tribello, M. Ceriotti, and M. Parrinello, *Using sketch-map coordinates to analyze and bias molecular dynamics simulations*, Proceedings of the National Academy of Science of the USA **109**, 5196 (2012).

[203] M. Ceriotti, G. A. Tribello, and M. Parrinello, *Demonstrating the Transferability and the Descriptive Power of Sketch-Map*, Journal of Chemical Theory and Computation **9**, 1521 (2013).

[204] A. P. Bartók, R. Kondor, and G. Csányi, *On representing chemical environments*, Physical Review B **87**, 184115 (2013).

[205] G. Montavon, M. Rupp, V. Gobre, A. Vazquez-Mayagoitia, K. Hansen, A. Tkatchenko, K.-R. Müller, and O. Anatole von Lilienfeld, *Machine learning of molecular electronic properties in chemical compound space*, New Journal of Physics **15**, 095003 (2013).

[206] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013).

[207] T. Hastie, R. Tibshirani, and J. Friedman, *The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Second Edition* (Springer, New York, 2009).

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

[209] O. A. von Lilienfeld, R. D. Lins, and U. Rothlisberger, *Variational particle number approach for rational compound design*, Physical Review Letters **95**, 153002 (2005).

[210] M. Rupp, *Machine learning for quantum mechanics in a nutshell*, International Journal of Quantum Chemistry **115**, 1058 (2015).

[211] M. Seeger, *Greedy forward selection in the informative vector machine*, Tech. rep., University of California at Berkeley (2004).

[212] A. Krause and D. Golovin, *Submodular function maximization*, in *Tractability: Practical Approaches to Hard Problems*, L. Bordeaux, Y. Hamadi, and P. Kohli, eds. (Cambridge University Press, 2014), p. 71.

[213] M. D. Wilkinson, M. Dumontier, I. J. Aalbersberg, G. Appleton, M. Axton, A. Baak, N. Blomberg, J.-W. Boiten, L. B. d. S. Santos, P. E. Bourne, J. Bouwman, A. J. Brookes, T. Clark, M. Crosas, I. Dillo, O. Dumon, S. Edmunds, C. T. Evelo, R. Finkers, A. Gonzalez-Beltran, A. J. G. Gray, P. Groth, C. Goble, J. S. Grethe, J. Heringa, P. A. C. t. Hoen, R. Hooft, T. Kuhn, R. Kok, J. Kok, S. J. Lusher, M. E. Martone, A. Mons, A. L. Packer, B. Persson, P. Rocca-Serra, M. Roos, R. v. Schaik, S.-A. Sansone, E. Schultes, T. Sengstag, T. Slater, G. Strawn, M. A. Swertz, M. Thompson, J. v. d. Lei, E. v. Mulligen, J. Velterop, A. Waagmeester, P. Wittenburg, K. Wolstencroft, J. Zhao, and B. Mons, *The FAIR Guiding Principles for scientific data management and stewardship*, Scientific Data **3**, 160018 (2016).

[214] J. E. Saal, S. Kirklin, M. Aykol, B. Meredig, and C. Wolverton, *Materials Design and Discovery with High-Throughput Density Functional Theory: The Open Quantum Materials Database (OQMD)*, The Journal of The Minerals, Metals & Materials Society (TMS) **65**, 1501 (2013).

[215] B. B. Van Aken, T. T. M. Palstra, and N. A. Spaldin, *The origin of ferroelectricity in magnetoelectric $YMnO_3$*, Nature Materials **3**, 164 (2004).

[216] A. Y. Birenbaum and C. Ederer, *Potentially multiferroic Aurivillius phase $Bi_5FeTi_3O_{15}$: Cation site preference, electric polarization, and magnetic coupling from first principles*, Physical Review B **90**, 214109 (2014).

[217] A. Y. Birenbaum and C. Ederer, *Controlling the cation distribution and electronic polarization with epitaxial strain in Aurivillius-phase $Bi_5FeTi_3O_{15}$*, Applied Physics Letters **108**, 082903 (2016).

[218] A. K. Yadav, C. T. Nelson, S. L. Hsu, Z. Hong, J. D. Clarkson, C. M. Schlepütz, A. R. Damodaran, P. Shafer, E. Arenholz, L. R. Dedon, D. Chen, A. Vishwanath, A. M. Minor, L. Q. Chen, J. F. Scott, L. W. Martin, and R. Ramesh, *Observation of polar vortices in oxide superlattices*, Nature **530**, 198 (2016).

[219] R. Guzmán, L. Maurel, E. Langenberg, A. R. Lupini, P. A. Algarabel, J. A. Pardo, and C. Magén, *Polar-Graded Multiferroic $SrMnO_3$ Thin Films*, Nano Letters **16**, 2221 (2016).

[220] A. B. Yankovich, B. Berkels, W. Dahmen, P. Binev, S. I. Sanchez, S. A. Bradley, A. Li, I. Szlufarska, and P. M. Voyles, *Picometre-precision analysis of scanning transmission electron microscopy images of platinum nanocatalysts*, Nature Communications **5**, 4155 (2014).

[221] R. J. Klingler, M. J. Chen, J. W. Rathke, and K. W. Kramarz, *Effect of Phosphines on the Thermodynamics of the Cobalt-Catalyzed Hydroformylation System*, Organometallics **26**, 352 (2007).

[222] J. M. Birbeck, A. Haynes, H. Adams, L. Damoense, and S. Otto, *Ligand Effects on Reactivity of Cobalt Acyl Complexes*, ACS Catalysis **2**, 2512 (2012).

[223] M. Ranocchiari and J. A. v. Bokhoven, *Catalysis by metal-organic frameworks: fundamentals and opportunities*, Physical Chemistry Chemical Physics **13**, 6388 (2011).

[224] N. Nosengo, *Can artificial intelligence create the next wonder material?*, Nature **533**, 22 (2016).

Annex 1 Publication list

All publications have been entered in NIRA, and are listed below, sorted by group leaders. We list publications either resulting directly from the NCCR (marked with a red hexagon) or with minor contributions from the NCCR. The following lists cover the period from May 1st, 2014 to January 31st, 2017.

1. Scientific articles in journals with peer review
2. Scientific articles in journals without peer review
3. Publications from lists 1 and 2 involving several groups

1. Scientific articles in journals with peer review

Group of Wanda Andreoni

- C. Ma, F. Pietrucci, and W. Andreoni
  Reaction dynamics of CO_2 in aqueous amines from ab initio molecular dynamics: 2-amino-2-methyl-1,3-propanediol (AMPD) compared to monoethanolamine (MEA)
  Theoretical Chemistry Accounts **135**, 60 (2016).
  Group(s): Andreoni / Project(s): VP2

W. Andreoni and F. Pietrucci
CO_2 capture in amine solutions: modelling and simulations with non-empirical methods
Journal of Physics: Condensed Matter **28**, 503003 (2016).
Group(s): Andreoni / Project(s): VP2

Group of Claudia Cancellieri

- F. Evangelisti, M. Stiefel, O. Guseva, R. P. Nia, R. Hauert, E. Hack, L. P. H. Jeurgens, F. Ambrosio, A. Pasquarello, P. Schmutz, and C. Cancellieri
  Electronic and structural characterization of barrier-type amorphous aluminium oxide
  Electrochimica Acta **224**, 503 (2017).
  Group(s): Cancellieri, Pasquarello / Project(s): VP2, PP7

Group of Michele Ceriotti

- S. De, F. Musil, T. Ingram, C. Baldauf, and M. Ceriotti
  Mapping and classifying molecules from a high-throughput structural database
  Journal of Cheminformatics **9**, 6 (2017).
  Group(s): Ceriotti / Project(s): HP5

- S. De, A. P. Bartók, G. Csányi, and M. Ceriotti
  Comparing molecules and solids across structural and alchemical space
  Physical Chemistry Chemical Physics **18**, 13754 (2016).
  Group(s): Ceriotti / Project(s): HP5

M. Rossi, P. Gasparotto, and M. Ceriotti
Anharmonic and Quantum Fluctuations in Molecular Crystals: A First-Principles Study of the Stability of Paracetamol
Physical Review Letters **117**, 115702 (2016).
Group(s): Ceriotti / Project(s): HP4

P. Gasparotto, A. A. Hassanali, and M. Ceriotti
Probing Defects and Correlations in the Hydrogen-Bond Network of ab Initio Water
Journal of Chemical Theory and Computation **12**, 1953 (2016).
Group(s): Ceriotti / Project(s): HP4

- V. Kapil, J. VandeVondele, and M. Ceriotti

Accurate molecular dynamics and nuclear quantum effects at low cost by multiple steps in real and imaginary time: Using density functional theory to accelerate wavefunction methods

The Journal of Chemical Physics **144**, 054111 (2016).

Group(s): Ceriotti, VandeVondele / Project(s): HP3,HP4

R. Petraglia, A. Nicolaï, M. D. Wodrich, M. Ceriotti, and C. Corminboeuf

Beyond Static Structures: Putting Forth REMD as a Tool to Solve Problems in Computational Organic Chemistry

Journal of Computational Chemistry **37**, 83 (2016).

Group(s): Ceriotti, Corminboeuf / Project(s): HP4

A. Ardevol, G. A. Tribello, M. Ceriotti, and M. Parrinello

Probing the Unfolded Configurations of a β-Hairpin Using Sketch-Map

Journal of Chemical Theory and Computation **11**, 1086 (2015).

Group(s): Ceriotti, Parrinello / Project(s): HP4

- P. Gasparotto and M. Ceriotti

Recognizing molecular patterns by machine learning: An agnostic structural definition of the hydrogen bond

The Journal of Chemical Physics **141**, 174110 (2014).

Group(s): Ceriotti / Project(s): HP4

Group of Volkan Cevher

- D. Carlson, Y.-P. Hsieh, E. Collins, L. Carin, and V. Cevher

Stochastic Spectral Descent for Discrete Graphical Models

IEEE Journal of Selected Topics in Signal Processing (2016), doi:10.1109/JSTSP.2015.2505684.

Group(s): Cevher, Koch / Project(s): HP5

A. Norouzi-Fard, A. Bazzi, I. Bogunovic, M. El Halabi, Y.-P. Hsieh, and V. Cevher

An Efficient Streaming Algorithm for the Submodular Cover Problem

in *Advances in Neural Information Processing Systems 29 (NIPS 2016)*, D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett., eds. (2016).

Group(s): Cevher / Project(s): HP5

- D. E. Carlson, E. Collins, Y.-P. Hsieh, L. Carin, and V. Cevher

Preconditioned Spectral Descent for Deep Learning

in *Advances in Neural Information Processing Systems 28 (NIPS 2015)*, C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, eds. (2015).

Group(s): Cevher, Koch / Project(s): HP5

Group of Clémence Corminboeuf

- M. Wodrich, M. Busch, and C. Corminboeuf

Accessing and predicting the kinetic profiles of homogeneous catalysts from volcano plots

Chemical Science **7**, 5723 (2016).

Group(s): Corminboeuf / Project(s): VP2

R. Petraglia, A. Nicolaï, M. D. Wodrich, M. Ceriotti, and C. Corminboeuf

Beyond Static Structures: Putting Forth REMD as a Tool to Solve Problems in Computational Organic Chemistry

Journal of Computational Chemistry **37**, 83 (2016).

Group(s): Ceriotti, Corminboeuf / Project(s): HP4

- M. Busch, M. Wodrich, and C. Corminboeuf

Linear Scaling Relationships and Volcano Plots in Homogeneous Catalysis ? Revisiting the Suzuki Reaction

Chemical Science **6**, 6754 (2015).

Group(s): Corminboeuf / Project(s): VP2

- G. Gryn'ova, M. Coote, and C. Corminboeuf

Theory and practice of uncommon molecular electronic configurations

WIREs Computational Molecular Science **5**, 440 (2015).

Group(s): Corminboeuf / Project(s): VP2

Group of Alessandro Curioni

P. Staar, M. Jiang, U. R. Hähner, T. C. Schulthess, and T. A. Maier

Interlaced coarse-graining for the dynamic cluster approximation

Physical Review B **93**, 165144 (2016).

Group(s): Curioni, Schulthess / Project(s): HP5

P. W. J. Staar, P. K. Barkoutsos, R. Istrate, A. C. I. Malossi, I. Tavernelli, N. Moll, H. Giefers, C. Hagleitner, C. Bekas, and A. Curioni

Stochastic matrix-function estimators: Scalable Big-Data kernels with high performance

in *2016 IEEE International Parallel and Distributed Processing Symposium (IPDPS)* (2016),

p. 812, doi:10.1109/IPDPS.2016.34.
Group(s): Curioni / Project(s): HP5

F. Franco de Carvalho and I. Tavernelli
Nonadiabatic dynamics with intersystem crossings: A time-dependent density functional theory implementation
The Journal of Chemical Physics **143**, 224105 (2015).
Group(s): Curioni / Project(s): VP2

- K. Meier, T. Laino, and A. Curioni
Solid-State Electrolytes: Revealing the Mechanisms of Li-Ion Conduction in Tetragonal and Cubic LLZO by First-Principles Calculations
The Journal of Physical Chemistry C **118**, 6668 (2014).
Group(s): Curioni / Project(s): VP2

Group of Antoine Georges

M. Kim, Y. Nomura, M. Ferrero, P. Seth, O. Parcollet, and A. Georges
Enhancing superconductivity in A_3C_{60} fullerides
Physical Review B **94**, 155152 (2016).
Group(s): Georges / Project(s): VP1

J. Mravlje and A. Georges
Thermopower and Entropy: Lessons from Sr_2RuO_4
Physical Review Letters **117**, 036401 (2016).
Group(s): Georges / Project(s): VP1

- M. Aichhorn, L. Pourovskii, P. Seth, V. Vildosola, M. Zingl, O. E. Peil, X. Deng, J. Mravlje, G. J. Kraberger, C. Martins, M. Ferrero, and O. Parcollet
TRIQS/DFTTools: A TRIQS application for ab initio calculations of correlated materials
Computer Physics Communications **204**, 200 (2016).
Group(s): Georges / Project(s): VP1

H. T. Dang, J. Mravlje, A. Georges, and A. J. Millis
Band Structure and Terahertz Optical Conductivity of Transition Metal Oxides: Theory and Application to $CaRuO_3$
Physical Review Letters **115**, 107003 (2015).
Group(s): Georges / Project(s): VP1

H. T. Dang, J. Mravlje, A. Georges, and A. J. Millis
Electronic correlations, magnetism, and Hund's rule coupling in the ruthenium perovskites $SrRuO_3$ and $CaRuO_3$
Physical Review B **91**, 195149 (2015).
Group(s): Georges / Project(s): VP1

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

- J. Ruppen, J. Teyssier, O. E. Peil, S. Catalano, M. Gibert, J. Mravlje, J.-M. Triscone, A. Georges, and D. van der Marel
Optical spectroscopy and the nature of the insulating state of rare-earth nickelates
Physical Review B **92**, 155145 (2015).
Group(s): Georges, van der Marel / Project(s): VP1, PP7

D. Stricker, J. Mravlje, C. Berthod, R. Fittipaldi, A. Vecchione, A. Georges, and D. van der Marel
Optical Response of Sr_2RuO_4 Reveals Universal Fermi-Liquid Scaling and Quasiparticles Beyond Landau Theory
Physical Review Letters **113**, 087404 (2014).
Group(s): Georges / Project(s): VP1

O. E. Peil, M. Ferrero, and A. Georges
Orbital polarization in strained $LaNiO_3$: Structural distortions and correlation effects
Physical Review B **90**, 045128 (2014).
Group(s): Georges / Project(s): VP1

Group of Stefan Goedecker

- G. Fisicaro, L. Genovese, O. Andreussi, N. Marzari, and S. Goedecker
A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments
The Journal of Chemical Physics **144**, 014103 (2016).
Group(s): Goedecker, Marzari / Project(s): HP3

- L. Zhu, M. Amsler, T. Fuhrer, B. Schaefer, S. Faraji, S. Rostami, S. A. Ghasemi, A. Sadeghi, M. Grauzinyte, C. Wolverton, and S. Goedecker
A fingerprint based metric for measuring similarities of crystalline structures
The Journal of Chemical Physics **144**, 034203 (2016).
Group(s): Goedecker / Project(s): HP4

- B. Schaefer and S. Goedecker
Computationally efficient characterization of potential energy surfaces based on fingerprint distances
The Journal of Chemical Physics **145**, 034101

(2016).

Group(s): Goedecker / Project(s): HP4

- J. A. Flores-Livas, M. Amsler, C. Heil, A. Sanna, L. Boeri, G. Profeta, C. Wolverton, S. Goedecker, and E. K. U. Gross
  Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure
  Physical Review B **93**, 020508 (2016).
  Group(s): Goedecker / Project(s): HP4

- K. Lejaeghere, G. Bihlmayer, T. Björkman, P. Blaha, S. Blügel, V. Blum, D. Caliste, I. E. Castelli, S. J. Clark, A. Dal Corso, S. de Gironcoli, T. Deutsch, J. K. Dewhurst, I. Di Marco, C. Draxl, M. Dulak, O. Eriksson, J. A. Flores-Livas, K. F. Garrity, L. Genovese, P. Giannozzi, M. Giantomassi, S. Goedecker, X. Gonze, O. Grånäs, E. K. U. Gross, A. Gulans, F. Gygi, D. R. Hamann, P. J. Hasnip, N. A. W. Holzwarth, D. Iuşan, D. B. Jochym, F. Jollet, D. Jones, G. Kresse, K. Koepernik, E. Küçükbenli, Y. O. Kvashnin, I. L. M. Locht, S. Lubeck, M. Marsman, N. Marzari, U. Nitzsche, L. Nordström, T. Ozaki, L. Paulatto, C. J. Pickard, W. Poelmans, M. I. J. Probert, K. Refson, M. Richter, G.-M. Rignanese, S. Saha, M. Scheffler, M. Schlipf, K. Schwarz, S. Sharma, F. Tavazza, P. Thunström, A. Tkatchenko, M. Torrent, D. Vanderbilt, M. J. van Setten, V. Van Speybroeck, J. M. Wills, J. R. Yates, G.-X. Zhang, and S. Cottenier
  Reproducibility in density functional theory calculations of solids
  Science **351**, 6280 (2016).
  Group(s): Goedecker, Marzari / Project(s): PP6, VP2

M. Amsler, S. Botti, M. A. L. Marques, T. J. Lenosky, and S. Goedecker
Low-density silicon allotropes for photovoltaic applications
Physical Review B **92**, 014101 (2015).
Group(s): Goedecker / Project(s): HP4

B. Schaefer, S. A. Ghasemi, S. Roy, and S. Goedecker
Stabilized quasi-Newton optimization of noisy potential energy surfaces
The Journal of Chemical Physics **142**, 034112 (2015).
Group(s): Goedecker / Project(s): HP4

Group of Jürg Hutter

F. H. Hodel and S. Luber
Redox-Inert Cations Enhancing Water Oxidation Activity: The Crucial Role of Flexibility
ACS Catalysis **6**, 6750 (2016).
Group(s): Hutter / Project(s): VP2

F. H. Hodel and S. Luber
What Influences the Water Oxidation Activity of a Bioinspired Molecular $Co_4^{II}O_4$ Cubane? An In-Depth Exploration of Catalytic Pathways
ACS Catalysis **6**, 1505 (2016).
Group(s): Hutter / Project(s): VP2

M. Schilling, G. R. Patzke, J. Hutter, and S. Luber
Computational Investigation and Design of Cobalt Aqua Complexes for Homogeneous Water Oxidation
The Journal of Physical Chemistry C **120**, 7966 (2016).
Group(s): Hutter / Project(s): VP2

G. Mette, D. Sutter, Y. Gurdal, S. Schnidrig, B. Probst, M. Iannuzzi, J. Hutter, R. Alberto, and J. Osterwalder
From porphyrins to pyrphyrins: adsorption study and metalation of a molecular catalyst on Au(111)
Nanoscale **8**, 7958 (2016).
Group(s): Hutter / Project(s): VP2

- G. Miceli, J. Hutter, and A. Pasquarello
  Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets
  Journal of Chemical Theory and Computation **12**, 3456 (2016).
  Group(s): Hutter, Pasquarello / Project(s): VP2,HP3

- J. Wilhelm, M. Del Ben, and J. Hutter
  GW in the Gaussian and Plane Waves Scheme with Application to Linear Acenes
  Journal of Chemical Theory and Computation **12**, 3623 (2016).
  Group(s): Hutter / Project(s): HP3

- J. Wilhelm, P. Seewald, M. Del Ben, and J. Hutter
  Large-Scale Cubic-Scaling Random Phase Approximation Correlation Energy Calculations Using a Gaussian Basis
  Journal of Chemical Theory and Computation **12**, 5851 (2016).
  Group(s): Hutter / Project(s): HP3

F. Evangelisti, R. Moré, F. Hodel, S. Luber, and G. R. Patzke

3d–4f $Co^{II}_3Ln(OR)_4$ Cubanes as Bio-Inspired Water Oxidation Catalysts

Journal of the American Chemical Society **137**, 11076 (2015).

Group(s): Hutter / Project(s): VP2

- Y. Gurdal, S. Luber, J. Hutter, and M. Iannuzzi
  Non-innocent adsorption of Co-pyrphyrin on rutile(110)

  Physical Chemistry Chemical Physics **17**, 22846 (2015).

  Group(s): Hutter / Project(s): VP2

- M. Del Ben, O. Schütt, T. Wentz, P. Messmer, J. Hutter, and J. VandeVondele
  Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution

  Computer Physics Communications **187**, 120 (2015).

  Group(s): Hutter, VandeVondele / Project(s): HP3

- M. Del Ben, J. Hutter, and J. VandeVondele
  Forces and stress in second order Møller-Plesset perturbation theory for condensed phase systems within the resolution-of-identity Gaussian and plane waves approach

  The Journal of Chemical Physics **143**, 102803 (2015).

  Group(s): Hutter, VandeVondele / Project(s): HP3

- M. Del Ben, J. Hutter, and J. VandeVondele
  Probing the structural and dynamical properties of liquid water with models including non-local electron correlation

  The Journal of Chemical Physics **143**, 054506 (2015).

  Group(s): Hutter, VandeVondele / Project(s): HP3

U. Borštnik, J. VandeVondele, V. Weber, and J. Hutter
Sparse matrix multiplication: The distributed block-compressed sparse row library

Parallel Computing **40**, 47 (2014).

Group(s): Hutter, VandeVondele / Project(s): HP3

Group of Christoph Koch

- A. Shaikhha, Y. Klonatos, L. Parreaux, L. Brown, M. Dashti, and C. Koch
  How to Architect a Query Compiler

  in *Proceedings of the 2016 International Conference on Management of Data* (ACM, New York, NY, USA, 2016), SIGMOD '16, p. 1907.

  Group(s): Koch / Project(s): HP5

I. Trummer and C. Koch
Multiple Query Optimization on the D-Wave 2X Adiabatic Quantum Computer

Proceedings of the VLDB Endowment **9**, 660 (2016), arXiv:1510.06437.

Group(s): Koch / Project(s): HP5

- D. Carlson, Y.-P. Hsieh, E. Collins, L. Carin, and V. Cevher
  Stochastic Spectral Descent for Discrete Graphical Models

  IEEE Journal of Selected Topics in Signal Processing (2016), doi:10.1109/JSTSP.2015.2505684.

  Group(s): Cevher, Koch / Project(s): HP5

- D. E. Carlson, E. Collins, Y.-P. Hsieh, L. Carin, and V. Cevher
  Preconditioned Spectral Descent for Deep Learning

  in *Advances in Neural Information Processing Systems 28 (NIPS 2015)*, C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, eds. (2015).

  Group(s): Cevher, Koch / Project(s): HP5

Group of Thomas Lippert

- W. Si, D. Pergolesi, F. Haydous, A. Fluri, A. Wokaun, and T. Lippert
  Investigating the behavior of various cocatalysts on $LaTaON_2$ photoanode for visible light water splitting

  Physical Chemistry Chemical Physics **19**, 656 (2017).

  Group(s): Lippert, Pergolesi / Project(s): PP7

Group of Nicola Marzari

Y. Hinuma, G. Pizzi, Y. Kumagai, F. Oba, and I. Tanaka
Band structure diagram paths based on crystallography

Computational Materials Science **128**, 140 (2017).

Group(s): Marzari / Project(s): PP6

- N. Marzari
  Materials modelling: The frontiers and the challenges

  Nature Materials **15**, 381 (2016).

  Group(s): Marzari / Project(s): VP2

- G. Pizzi, M. Gibertini, E. Dib, N. Marzari, G. Iannaccone, and G. Fiori
  Performance of arsenene and antimonene double-gate MOSFETs from first principles

Nature Communications **7**, 12585 (2016).
Group(s): Marzari / Project(s): VP2

T. Y. Kim, C.-H. Park, and N. Marzari
The Electronic Thermal Conductivity of Graphene
Nano Letters **16**, 2439 (2016).
Group(s): Marzari / Project(s): VP2

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

J. Hu, G. M. Vanacore, A. Cepellotti, N. Marzari, and A. H. Zewail
Rippling ultrafast dynamics of suspended 2D monolayers, graphene
Proceedings of the National Academy of Science of the USA **113**, E6555 (2016).
Group(s): Marzari / Project(s): VP2

G. Fisicaro, L. Genovese, O. Andreussi, N. Marzari, and S. Goedecker
A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments
The Journal of Chemical Physics **144**, 014103 (2016).
Group(s): Goedecker, Marzari / Project(s): HP3

N. L. Nguyen, G. Borghi, A. Ferretti, and N. Marzari
First-Principles Photoemission Spectroscopy of DNA and RNA Nucleobases from Koopmans-Compliant Functionals
Journal of Chemical Theory and Computation **12**, 3948 (2016).
Group(s): Marzari / Project(s): HP3

M. M. Montemore, O. Andreussi, and J. W. Medlin
Hydrocarbon adsorption in an aqueous environment: A computational study of alkyls on Cu(111)
The Journal of Chemical Physics **145**, 074702 (2016).
Group(s): Marzari / Project(s): HP4

L. Sementa, O. Andreussi, W. A. Goddard, and A. Fortunelli
Catalytic activity of Pt_{38} in the oxygen reduction reaction from first-principles simulations
Catalysis Science & Technology **6**, 6901 (2016).
Group(s): Marzari / Project(s): HP4

G. W. Mann, K. Lee, M. Cococcioni, B. Smit, and J. B. Neaton
First-principles Hubbard U approach for small molecule binding in metal-organic frameworks
The Journal of Chemical Physics **144**, 174104 (2016).
Group(s): Marzari, Smit / Project(s): HP4

K. Lejaeghere, G. Bihlmayer, T. Björkman, P. Blaha, S. Blügel, V. Blum, D. Caliste, I. E. Castelli, S. J. Clark, A. Dal Corso, S. de Gironcoli, T. Deutsch, J. K. Dewhurst, I. Di Marco, C. Draxl, M. Dulak, O. Eriksson, J. A. Flores-Livas, K. F. Garrity, L. Genovese, P. Giannozzi, M. Giantomassi, S. Goedecker, X. Gonze, O. Grånäs, E. K. U. Gross, A. Gulans, F. Gygi, D. R. Hamann, P. J. Hasnip, N. A. W. Holzwarth, D. Iuşan, D. B. Jochym, F. Jollet, D. Jones, G. Kresse, K. Koepernik, E. Küçükbenli, Y. O. Kvashnin, I. L. M. Locht, S. Lubeck, M. Marsman, N. Marzari, U. Nitzsche, L. Nordström, T. Ozaki, L. Paulatto, C. J. Pickard, W. Poelmans, M. I. J. Probert, K. Refson, M. Richter, G.-M. Rignanese, S. Saha, M. Scheffler, M. Schlipf, K. Schwarz, S. Sharma, F. Tavazza, P. Thunström, A. Tkatchenko, M. Torrent, D. Vanderbilt, M. J. van Setten, V. Van Speybroeck, J. M. Wills, J. R. Yates, G.-X. Zhang, and S. Cottenier
Reproducibility in density functional theory calculations of solids
Science **351**, 6280 (2016).
Group(s): Goedecker, Marzari / Project(s): PP6, VP2

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

M. Gibertini and N. Marzari
Emergence of One-Dimensional Wires of Free Carriers in Transition-Metal-Dichalcogenide Nanostructures
Nano Letters **15**, 6229 (2015).
Group(s): Marzari / Project(s): VP2, VP1

Y. Krupskaya, M. Gibertini, N. Marzari, and A. F. Morpurgo
Band-Like Electron Transport with Record-High Mobility in the TCNQ Family
Advanced Materials **27**, 2453 (2015).
Group(s): Marzari / Project(s): VP2

D. Dumcenco, D. Ovchinnikov, K. Marinov, P. Lazić, M. Gibertini, N. Marzari, O. L. Sanchez, Y.-C. Kung, D. Krasnozhon, M.-W. Chen, S. Bertolazzi,

P. Gillet, A. Fontcuberta i Morral, A. Radenovic, and A. Kis
Large-Area Epitaxial Mono layer MoS_2
ACS Nano **9**, 4611 (2015).
Group(s): Marzari / Project(s): VP2

A. Cepellotti, G. Fugallo, L. Paulatto, M. Lazzeri, F. Mauri, and N. Marzari
Phonon hydrodynamics in two-dimensional materials
Nature Communications **6**, 6400 (2015).
Group(s): Marzari / Project(s): VP2

D. Dragoni, D. Ceresoli, and N. Marzari
Thermoelastic properties of α-iron from first-principles
Physical Review B **91**, 104105 (2015).
Group(s): Marzari / Project(s): VP2

X. Cheng, E. Fabbri, M. Nachtegaal, I. E. Castelli, M. El Kazzi, R. Haumont, N. Marzari, and T. J. Schmidt
Oxygen Evolution Reaction on $La_{1-x}Sr_xCoO_3$ Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties
Chemistry of Materials **27**, 7662 (2015).
Group(s): Marzari, Schmidt / Project(s): PP7, VP2

I. Timrov, O. Andreussi, A. Biancardi, N. Marzari, and S. Baroni
Self-consistent continuum solvation for optical absorption of complex molecular systems in solution
The Journal of Chemical Physics **142**, 034111 (2015).
Group(s): Marzari / Project(s): HP3

X. Qian, P. Umari, and N. Marzari
First-principles investigation of organic photovoltaic materials C_{60}, C_{70}, $[C_{60}]$PCBM, and bis-$[C_{60}]$PCBM using a many-body G_0W_0-Lanczos approach
Physical Review B **91**, 245105 (2015).
Group(s): Marzari / Project(s): HP3

N. L. Nguyen, G. Borghi, A. Ferretti, I. Dabo, and N. Marzari
First-Principles Photoemission Spectroscopy and Orbital Tomography in Molecules from Koopmans-Compliant Functionals
Physical Review Letters **114**, 166405 (2015).
Group(s): Marzari / Project(s): HP3

G. Borghi, C.-H. Park, N. L. Nguyen, A. Ferretti, and N. Marzari
Variational minimization of orbital-density-dependent functionals
Physical Review B **91**, 155112 (2015).
Group(s): Marzari / Project(s): HP3

N. Bonnet, I. Dabo, and N. Marzari
Chemisorbed Molecules under Potential Bias: Detailed Insights from First-Principles Vibrational Spectroscopies
Electrochimica Acta **121**, 210 (2014).
Group(s): Marzari / Project(s): VP2

O. Andreussi and N. Marzari
Electrostatics of solvated systems in periodic boundary conditions
Physical Review B **90**, 245101 (2014).
Group(s): Marzari / Project(s): VP2

M. Gibertini, G. Pizzi, and N. Marzari
Engineering polar discontinuities in honeycomb lattices
Nature Communications **5**, 5157 (2014).
Group(s): Marzari / Project(s): VP2

M. Gibertini, F. M. D. Pellegrino, N. Marzari, and M. Polini
Spin-resolved optical conductivity of two-dimensional group-VIB transition-metal dichalcogenides
Physical Review B **90**, 245411 (2014).
Group(s): Marzari / Project(s): VP2

N. Bonnet and N. Marzari
Static Dielectric Permittivity of Ice from First Principles
Physical Review Letters **113**, 245501 (2014).
Group(s): Marzari / Project(s): VP2

G. Fugallo, A. Cepellotti, L. Paulatto, M. Lazzeri, N. Marzari, and F. Mauri
Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths
Nano Letters **14**, 6109 (2014).
Group(s): Marzari / Project(s): VP2,PP6

A. Ferretti, I. Dabo, M. Cococcioni, and N. Marzari
Bridging density-functional and many-body perturbation theory: Orbital-density dependence in electronic-structure functionals
Physical Review B **89**, 195134 (2014).
Group(s): Marzari / Project(s): HP3,VP2

I. Dabo, A. Ferretti, and N. Marzari
Piecewise Linearity and Spectroscopic Properties from Koopmans-Compliant Functionals
Topics in Current Chemistry **347**, 193 (2014).
Group(s): Marzari / Project(s): HP3,VP2

G. Borghi, A. Ferretti, N. L. Nguyen, I. Dabo, and N. Marzari

Koopmans-compliant functionals and their performance against reference molecular data

Physical Review B **90**, 075135 (2014).

Group(s): Marzari / Project(s): HP3,VP2

C.-H. Park, N. Bonini, T. Sohier, G. Samsonidze, B. Kozinsky, M. Calandra, F. Mauri, and N. Marzari

Electron-Phonon Interactions and the Intrinsic Electrical Resistivity of Graphene

Nano Letters **14**, 1113 (2014).

Group(s): Marzari / Project(s): PP6,VP2

T. Sohier, M. Calandra, C.-H. Park, N. Bonini, N. Marzari, and F. Mauri

Phonon-limited resistivity of graphene by first-principles calculations: Electron-phonon interactions, strain-induced gauge field, and Boltzmann equation

Physical Review B **90**, 125414 (2014).

Group(s): Marzari / Project(s): PP6,VP2

G. Pizzi, D. Volja, B. Kozinsky, M. Fornari, and N. Marzari

BoltzWann: *A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis*

Computer Physics Communications **185**, 422 (2014).

Group(s): Marzari / Project(s): PP6

S. Bruzzone, G. Iannaccone, N. Marzari, and G. Fiori

An Open-Source Multiscale Framework for the Simulation of Nanoscale Devices

IEEE Transactions on Electron Devices **61**, 48 (2014).

Group(s): Marzari / Project(s): PP6

G. Pizzi, D. Volja, B. Kozinsky, M. Fornari, and N. Marzari

An updated version of BoltzWann: *A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis*

Computer Physics Communications **185**, 2311 (2014).

Group(s): Marzari / Project(s): PP6

A. A. Mostofi, J. R. Yates, G. Pizzi, Y.-S. Lee, I. Souza, D. Vanderbilt, and N. Marzari

An updated version of `wannier90`*: A tool for obtaining maximally-localised Wannier functions*

Computer Physics Communications **185**, 2309 (2014).

Group(s): Marzari / Project(s): PP6

Group of Michele Parrinello

- M. Nava, F. Palazzesi, C. Perego, and M. Parrinello

  Dimer metadynamics

  Journal of Chemical Theory and Computation (2017), doi:10.1021/acs.jctc.6b00691.

  Group(s): Parrinello / Project(s): HP4

- O. Valsson, P. Tiwary, and M. Parrinello

  Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint

  Annual Review of Physical Chemistry **67**, 159 (2016).

  Group(s): Parrinello / Project(s): HP4

- P. M. Piaggi, O. Valsson, and M. Parrinello

  A variational approach to nucleation simulation

  Faraday Discussions **195**, 557 (2016).

  Group(s): Parrinello / Project(s): HP4

- J. McCarty, O. Valsson, and M. Parrinello

  Bespoke Bias for Obtaining Free Energy Differences within Variationally Enhanced Sampling

  Journal of Chemical Theory and Computation **12**, 2162 (2016).

  Group(s): Parrinello / Project(s): HP4

P. Shaffer, O. Valsson, and M. Parrinello

Hierarchical Protein Free Energy Landscapes from Variationally Enhanced Sampling

Journal of Chemical Theory and Computation **12**, 5751 (2016).

Group(s): Parrinello / Project(s): HP4

- P. Shaffer, O. Valsson, and M. Parrinello

  Enhanced, targeted sampling of high-dimensional free-energy landscapes using variationally enhanced sampling, with an application to chignolin

  Proceedings of the National Academy of Science of the USA **113**, 1150 (2016).

  Group(s): Parrinello / Project(s): HP4

- C. Perego, F. Giberti, and M. Parrinello

  Chemical potential calculations in dense liquids using metadynamics

  The European Physical Journal – Special Topics **225**, 1621 (2016).

  Group(s): Parrinello / Project(s): HP4

- M. Salvalaglio, P. Tiwary, G. M. Maggioni, M. Mazzotti, and M. Parrinello

Overcoming time scale and finite size limitations to compute nucleation rates from small scale well tempered metadynamics simulations

The Journal of Chemical Physics **145**, 211925 (2016).

Group(s): Parrinello / Project(s): HP4

- M. Salvalaglio, M. Mazzotti, and M. Parrinello
  Urea homogeneous nucleation mechanism is solvent dependent

  Faraday Discussions (2015), doi:10.1039/C4FD00235K.

  Group(s): Parrinello / Project(s): HP4

- O. Valsson and M. Parrinello
  Well-Tempered Variational Approach to Enhanced Sampling

  Journal of Chemical Theory and Computation **11**, 1996 (2015).

  Group(s): Parrinello / Project(s): HP4

A. Ardevol, G. A. Tribello, M. Ceriotti, and M. Parrinello
Probing the Unfolded Configurations of a β-Hairpin Using Sketch-Map

Journal of Chemical Theory and Computation **11**, 1086 (2015).

Group(s): Ceriotti, Parrinello / Project(s): HP4

- J. McCarty, O. Valsson, P. Tiwary, and M. Parrinello
  Variationally Optimized Free-Energy Flooding for Rate Calculation

  Physical Review Letters **115**, 070601 (2015).

  Group(s): Parrinello / Project(s): HP4

- M. Salvalaglio, C. Perego, F. Giberti, M. Mazzotti, and M. Parrinello
  Molecular-dynamics simulations of urea nucleation from aqueous solution

  Proceedings of the National Academy of Science of the USA **112**, E6 (2015).

  Group(s): Parrinello / Project(s): HP4

- C. Perego, M. Salvalaglio, and M. Parrinello
  Molecular dynamics simulations of solutions at constant chemical potential

  The Journal of Chemical Physics **142**, 144113 (2015).

  Group(s): Parrinello / Project(s): HP4

- O. Valsson and M. Parrinello
  Variational Approach to Enhanced Sampling and Free Energy Calculations

  Physical Review Letters **113**, 090601 (2014).

  Group(s): Parrinello / Project(s): HP4

Group of Alfredo Pasquarello

- F. Evangelisti, M. Stiefel, O. Guseva, R. P. Nia, R. Hauert, E. Hack, L. P. H. Jeurgens, F. Ambrosio, A. Pasquarello, P. Schmutz, and C. Cancellieri
  Electronic and structural characterization of barrier-type amorphous aluminium oxide

  Electrochimica Acta **224**, 503 (2017).

  Group(s): Cancellieri, Pasquarello / Project(s): VP2, PP7

- Z. Guo, F. Ambrosio, and A. Pasquarello
  Oxygen defects in amorphous Al_2O_3: A hybrid functional study

  Applied Physics Letters **109**, 062903 (2016).

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

- G. Miceli, J. Hutter, and A. Pasquarello
  Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets

  Journal of Chemical Theory and Computation **12**, 3456 (2016).

  Group(s): Hutter, Pasquarello / Project(s): VP2,HP3

- W. Chen, F. Ambrosio, G. Miceli, and A. Pasquarello
  Ab initio electronic structure of liquid water

  Physical Review Letters **117**, 186401 (2016).

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

- F. Ambrosio, G. Miceli, and A. Pasquarello
  Structural, dynamical, and electronic properties of liquid water: A hybrid functional study

  The Journal of Physical Chemistry B **120**, 7456 (2016).

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

W. Chen and A. Pasquarello
First-principles determination of defect energy levels through hybrid density functionals and GW

Journal of Physics: Condensed Matter **27**, 133202 (2015).

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

W. Chen and A. Pasquarello
Accurate band gaps of extended systems via efficient vertex corrections in GW

Physical Review B **92**, 041115 (2015).

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

- G. Miceli, S. de Gironcoli, and A. Pasquarello
  Isobaric first-principles molecular dynamics of liquid water with nonlocal van der Waals interactions

  The Journal of Chemical Physics **142**, 034501

(2015).

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

- F. Ambrosio, G. Miceli, and A. Pasquarello
  Redox levels in aqueous solution: Effect of van der Waals interactions and hybrid functionals
  The Journal of Chemical Physics **143**, 244508 (2015).
  Group(s): Pasquarello / Project(s): VP2

W. Chen and A. Pasquarello
Band-edge positions in GW: Effects of starting point and self-consistency
Physical Review B **90**, 165133 (2014).
Group(s): Pasquarello / Project(s): VP2

Group of Daniele Passerone

S. Kawai, A. Benassi, E. Gnecco, H. Söde, R. Pawlak, X. Feng, K. Müllen, D. Passerone, C. A. Pignedoli, P. Ruffieux, R. Fasel, and E. Meyer
Superlubricity of graphene nanoribbons on gold surfaces
Science **351**, 957 (2016).
Group(s): Passerone / Project(s): VP2

A. Basagni, G. Vasseur, C. A. Pignedoli, M. Vilas-Varela, D. Peña, L. Nicolas, L. Vitali, J. Lobo-Checa, D. G. de Oteyza, F. Sedona, M. Casarin, J. E. Ortega, and M. Sambi
Tunable Band Alignment with Unperturbed Carrier Mobility of On-Surface Synthesized Organic Semiconducting Wires
ACS Nano **10**, 2644 (2016).
Group(s): Passerone / Project(s): VP2

- P. Ruffieux, S. Wang, B. Yang, C. Sánchez-Sánchez, J. Liu, T. Dienel, L. Talirz, P. Shinde, C. A. Pignedoli, D. Passerone, T. Dumslaff, X. Feng, K. Müllen, and R. Fasel
  On-surface synthesis of graphene nanoribbons with zigzag edge topology
  Nature **531**, 489 (2016).
  Group(s): Passerone / Project(s): VP2

- S. Wang, L. Talirz, C. A. Pignedoli, X. Feng, K. Müllen, R. Fasel, and P. Ruffieux
  Giant edge state splitting at atomically precise graphene zigzag edges
  Nature Communications **7**, 11507 (2016).
  Group(s): Passerone / Project(s): VP2

M. D. Rossell, P. Agrawal, A. Borgschulte, C. Hébert, D. Passerone, and R. Erni
Direct Evidence of Surface Reduction in Monoclinic $BiVO_4$
Chemistry of Materials **27**, 3593 (2015).
Group(s): Passerone / Project(s): VP2

- A. Basagni, F. Sedona, C. A. Pignedoli, M. Cattelan, L. Nicolas, M. Casarin, and M. Sambi
  Molecules-Oligomers-Nanowires-Graphene Nanoribbons: A Bottom-Up Stepwise On-Surface Covalent Synthesis Preserving Long-Range Order
  Journal of the American Chemical Society **137**, 1802 (2015).
  Group(s): Passerone / Project(s): VP2

- H. Söde, L. Talirz, O. Gröning, C. A. Pignedoli, R. Berger, X. Feng, K. Müllen, R. Fasel, and P. Ruffieux
  Electronic band dispersion of graphene nanoribbons via Fourier-transformed scanning tunneling spectroscopy
  Physical Review B **91**, 045429 (2015).
  Group(s): Passerone / Project(s): VP2

R. Gaspari, R. Erni, Y. Arroyo, M. Parlinska-Wojtan, J. Dshemuchadse, C. A. Pignedoli, D. Passerone, P. Schmutz, and A. Beni
Real space crystallography of a complex metallic alloy: high-angle annular dark-field scanning transmission electron microscopy of o-Al_4(Cr,Fe)
Journal of Applied Crystallography **47**, 1026 (2014).
Group(s): Passerone / Project(s): VP2

R. Jaafar, C. A. Pignedoli, G. Bussi, K. Aït-Mansour, O. Gröning, T. Amaya, T. Hirao, R. Fasel, and P. Ruffieux
Bowl Inversion of Surface-Adsorbed Sumanene
Journal of the American Chemical Society **136**, 13666 (2014).
Group(s): Passerone / Project(s): VP2

J. Prinz, C. A. Pignedoli, Q. S. Stöckl, M. Armbrüster, H. Brune, O. Gröning, R. Widmer, and D. Passerone
Adsorption of Small Hydrocarbons on the Three-Fold PdGa Surfaces: The Road to Selective Hydrogenation
Journal of the American Chemical Society **136**, 11792 (2014).
Group(s): Passerone / Project(s): VP2

A. Benassi, A. Vanossi, C. A. Pignedoli, D. Passerone, and E. Tosatti

Does rotational melting make molecular crystal surfaces more slippery?

Nanoscale **6**, 13163 (2014).

Group(s): Passerone / Project(s): VP2

R. Denk, M. Hohage, P. Zeppenfeld, J. Cai, C. A. Pignedoli, H. Söde, R. Fasel, X. Feng, K. Müllen, S. Wang, D. Prezzi, A. Ferretti, A. Ruini, E. Molinari, and P. Ruffieux

Exciton-dominated optical response of ultra-narrow graphene nanoribbons

Nature Communications **5**, 4253 (2014).

Group(s): Passerone / Project(s): VP2

J. Cai, C. A. Pignedoli, L. Talirz, P. Ruffieux, H. Söde, L. Liang, V. Meunier, R. Berger, R. Li, X. Feng, K. Müllen, and R. Fasel

Graphene nanoribbon heterojunctions

Nature Nanotechnology **9**, 896 (2014).

Group(s): Passerone / Project(s): VP2

C. Karageorgaki, D. Passerone, and K.-H. Ernst

Chiral reconstruction of Cu(110) after adsorption of fumaric acid

Surface Science **629**, 75 (2014).

Group(s): Passerone / Project(s): VP2

D. J. Adams, S. Chappellet, F. Lincker, M. Ibn-Elhaj, B. Watts, M. Iannuzzi, D. S. Jung, C. A. Pignedoli, and D. Passerone

Identifying Photoreaction Products in Cinnamate-Based Photoalignment Materials

The Journal of Physical Chemistry C **118**, 15422 (2014).

Group(s): Passerone / Project(s): VP2

J. Prinz, R. Gaspari, Q. S. Stöckl, P. Gille, M. Armbrüster, H. Brune, O. Gröning, C. A. Pignedoli, D. Passerone, and R. Widmer

Ensemble Effect Evidenced by CO Adsorption on the 3-Fold PdGa Surfaces

The Journal of Physical Chemistry C **118**, 12260 (2014).

Group(s): Passerone / Project(s): VP2

Group of Daniele Pergolesi

- W. Si, D. Pergolesi, F. Haydous, A. Fluri, A. Wokaun, and T. Lippert

  Investigating the behavior of various cocatalysts on $LaTaON_2$ photoanode for visible light water splitting

  Physical Chemistry Chemical Physics **19**, 656 (2017).

  Group(s): Lippert, Pergolesi / Project(s): PP7

Group of Marco Ranocchiari

M. Taddei, D. Tiana, N. Casati, J. A. van Bokhoven, B. Smit, and M. Ranocchiari

Mixed-linker UiO-66: structure-property relationships revealed by a combination of high-resolution powder X-ray diffraction and density functional theory calculations

Physical Chemistry Chemical Physics **19**, 1551 (2017).

Group(s): Ranocchiari, Smit / Project(s): VP2

Group of Ursula Röthlisberger

E. Brunk, M. A. S. Perez, P. Athri, and U. Rothlisberger

Genetic-Algorithm-Based Optimization of a Peptidic Scaffold for Sequestration and Hydration of CO_2

ChemPhysChem **17**, 3831 (2016).

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

- C. Yi, J. Luo, S. Meloni, A. Boziki, N. Ashari-Astani, C. Grätzel, S. M. Zakeeruddin, U. Röthlisberger, and M. Grätzel

  Entropic stabilization of mixed A-cation ABX_3 metal halide perovskites for high performance perovskite solar cells

  Energy & Environmental Science **9**, 656 (2016).

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

- S. Meloni, G. Palermo, N. Ashari-Astani, M. Grätzel, and U. Rothlisberger

  Valence and conduction band tuning in halide perovskites for solar cell applications

  Journal of Materials Chemistry A **4**, 15997 (2016).

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

- S. Mathew, N. A. Astani, B. F. E. Curchod, J. H. Delcamp, M. Marszalek, J. Frey, U. Rothlisberger, M. K. Nazeeruddin, and M. Grätzel

  Synthesis, characterization and ab initio *investigation of a panchromatic ullazine-porphyrin photosensitizer for dye-sensitized solar cells*

  Journal of Materials Chemistry A **4**, 2332 (2016).

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

- S. Meloni, T. Moehl, W. Tress, M. Franckevičius, M. Saliba, Y. H. Lee, P. Gao, M. K. Nazeeruddin, S. M.

ZAKEERUDDIN, U. ROTHLISBERGER, AND M. GRAETZEL
Ionic polarization-induced current-voltage hysteresis in $CH_3NH_3PbX_3$ perovskite solar cells
Nature Communications **7**, 10334 (2016).
Group(s): Röthlisberger / Project(s): VP2

- M. I. DAR, G. JACOPIN, S. MELONI, A. MATTONI, N. ARORA, A. BOZIKI, S. M. ZAKEERUDDIN, U. ROTHLISBERGER, AND M. GRÄTZEL
Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites
Science Advances **2**, e1601156 (2016).
Group(s): Röthlisberger / Project(s): VP2

- W. TRESS, B. BEYER, N. ASHARI ASTANI, F. GAO, S. MELONI, AND U. ROTHLISBERGER
Extended Intermolecular Interactions Governing Photocurrent-Voltage Relations in Ternary Organic Solar Cells
The Journal of Physical Chemistry Letters **7**, 3936 (2016).
Group(s): Röthlisberger / Project(s): VP2

- K. VOÏTCHOVSKY, N. ASHARI ASTANI, I. TAVERNELLI, N. TÉTREAULT, U. ROTHLISBERGER, F. STELLACCI, M. GRÄTZEL, AND H. A. HARMS
In Situ Mapping of the Molecular Arrangement of Amphiphilic Dye Molecules at the TiO_2 Surface of Dye-Sensitized Solar Cells
ACS Applied Materials & Interfaces **7**, 10834 (2015).
Group(s): Röthlisberger / Project(s): VP2

E. BRUNK AND U. ROTHLISBERGER
Mixed Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of Biological Systems in Ground and Electronically Excited States
Chemical Reviews **115**, 6217 (2015).
Group(s): Röthlisberger / Project(s): VP2

E. BOZKURT, N. ASHARI, N. BROWNING, E. BRUNK, P. CAMPOMANES, M. A. S. PEREZ, AND U. ROTHLISBERGER
Lessons from Nature: Computational Design of Biomimetic Compounds and Processes
CHIMIA **68**, 642 (2014).
Group(s): Röthlisberger / Project(s): VP2

- S. MATHEW, A. YELLA, P. GAO, R. HUMPHRY-BAKER, B. F. E. CURCHOD, N. ASHARI-ASTANI, I. TAVERNELLI, U. ROTHLISBERGER, M. K. NAZEERUDDIN, AND M. GRÄTZEL
Dye-sensitized solar cells with 13% efficiency achieved through the molecular engineering of porphyrin sensitizers
Nature Chemistry **6**, 242 (2014).
Group(s): Röthlisberger / Project(s): VP2

Group of Thomas J. Schmidt

- X. CHENG, E. FABBRI, M. NACHTEGAAL, I. E. CASTELLI, M. EL KAZZI, R. HAUMONT, N. MARZARI, AND T. J. SCHMIDT
Oxygen Evolution Reaction on $La_{1-x}Sr_xCoO_3$ Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties
Chemistry of Materials **27**, 7662 (2015).
Group(s): Marzari, Schmidt / Project(s): PP7, VP2

Group of Thorsten Schmitt

X. LU, D. E. MCNALLY, M. MORETTI SALA, J. TERZIC, M. H. UPTON, D. CASA, G. INGOLD, G. CAO, AND T. SCHMITT
Doping Evolution of Magnetic Order and Magnetic Excitations in $(Sr_{1-x}La_x)_3Ir_2O_7$
Physical Review Letters **118**, 027202 (2017).
Group(s): Schmitt / Project(s): PP7

Group of Thomas Schulthess

- S. M. GRIFFIN, P. STAAR, T. C. SCHULTHESS, M. TROYER, AND N. A. SPALDIN
A bespoke single-band Hubbard model material
Physical Review B **93**, 075115 (2016).
Group(s): Schulthess, Spaldin, Troyer / Project(s): VP1

P. STAAR, M. JIANG, U. R. HÄHNER, T. C. SCHULTHESS, AND T. A. MAIER
Interlaced coarse-graining for the dynamic cluster approximation
Physical Review B **93**, 165144 (2016).
Group(s): Curioni, Schulthess / Project(s): HP5

T. C. SCHULTHESS
Programming revisited
Nature Physics **11**, 369 (2015).
Group(s): Schulthess / Project(s): PP6

R. SOLCÀ, A. KOZHEVNIKOV, A. HAIDAR, S. TOMOV, J. DONGARRA, AND T. C. SCHULTHESS
Efficient implementation of quantum materials simulations on distributed CPU-GPU systems
in *SC'15, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis* (ACM, New York, 2015), article No. 10, doi:10.1145/2807591.2807654.
Group(s): Schulthess / Project(s): PP6

P. Staar, T. Maier, and T. C. Schulthess
Two-particle correlations in a dynamic cluster approximation with continuous momentum dependence: Superconductivity in the two-dimensional Hubbard model
Physical Review B **89**, 195133 (2014).
Group(s): Schulthess / Project(s): PP6

I.-H. Chu, A. Kozhevnikov, T. C. Schulthess, and H.-P. Cheng
All-electron GW quasiparticle band structures of group 14 nitride compounds
The Journal of Chemical Physics **141**, 044709 (2014).
Group(s): Schulthess / Project(s): PP6

Group of Ming Shi

N. Xu, H. Ding, and M. Shi
Spin- and angle-resolved photoemission on the topological Kondo insulator candidate: SmB_6
Journal of Physics: Condensed Matter **28**, 363001 (2016).
Group(s): Shi / Project(s): PP7

- N. Xu, H. M. Weng, B. Q. Lv, C. E. Matt, J. Park, F. Bisti, V. N. Strocov, D. Gawryluk, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, G. Autès, O. V. Yazyev, Z. Fang, X. Dai, T. Qian, J. Mesot, H. Ding, and M. Shi
Observation of Weyl nodes and Fermi arcs in tantalum phosphide
Nature Communications **7**, 11006 (2016).
Group(s): Shi, Yazyev / Project(s): PP7, VP1

Group of Berend Smit

S. Jawahery, C. M. Simon, E. Braun, M. Witman, D. Tiana, B. Vlaisavljevich, and B. Smit
Adsorbate-induced lattice deformation in IRMOF-74 series
Nature Communications **8**, 13945 (2017).
Group(s): Smit / Project(s): VP2

M. Taddei, D. Tiana, N. Casati, J. A. van Bokhoven, B. Smit, and M. Ranocchiari
Mixed-linker UiO-66: structure-property relationships revealed by a combination of high-resolution powder X-ray diffraction and density functional theory calculations
Physical Chemistry Chemical Physics **19**, 1551 (2017).
Group(s): Ranocchiari, Smit / Project(s): VP2

G. W. Mann, K. Lee, M. Cococcioni, B. Smit, and J. B. Neaton
First-principles Hubbard U approach for small molecule binding in metal-organic frameworks
The Journal of Chemical Physics **144**, 174104 (2016).
Group(s): Marzari, Smit / Project(s): HP4

Group of Nicola Spaldin

- S. M. Griffin, P. Staar, T. C. Schulthess, M. Troyer, and N. A. Spaldin
A bespoke single-band Hubbard model material
Physical Review B **93**, 075115 (2016).
Group(s): Schulthess, Spaldin, Troyer / Project(s): VP1

- G. Sclauzero, K. Dymkowski, and C. Ederer
Tuning the metal-insulator transition in d^1 and d^2 perovskites by epitaxial strain: a first principles-based study
Physical Review B **94**, 245109 (2016).
Group(s): Spaldin / Project(s): VP1

- M. Morin, A. Scaramucci, M. Bartkowiak, E. Pomjakushina, G. Deng, D. Sheptyakov, L. Keller, J. Rodriguez-Carvajal, N. A. Spaldin, M. Kenzelmann, K. Conder, and M. Medarde
Incommensurate magnetic structure, Fe/Cu chemical disorder, and magnetic interactions in the high-temperature multiferroic $YBaCuFeO_5$
Physical Review B **91**, 064408 (2015).
Group(s): Kenzelmann, Medarde, Spaldin / Project(s): VP1, PP7

- G. Sclauzero and C. Ederer
Structural and electronic properties of epitaxially strained $LaVO_3$ from density functional theory and dynamical mean-field theory
Physical Review B **92**, 235112 (2015).
Group(s): Spaldin / Project(s): VP1

N. S. Fedorova, C. Ederer, N. A. Spaldin, and A. Scaramucci
Biquadratic and ring exchange interactions in orthorhombic perovskite manganites
Physical Review B **91**, 165122 (2015).
Group(s): Spaldin / Project(s): VP1

J. A. Heuver, A. Scaramucci, Y. Blickenstorfer, S. Matzen, N. A. Spaldin, C. Ederer, and B. Noheda
Strain-induced magnetic anisotropy in epitaxial thin films of the spinel $CoCr_2O_4$
Physical Review B **92**, 214429 (2015).
Group(s): Spaldin / Project(s): VP1

Group of Matthias Troyer

- D. Gresch, G. Autès, O. V. Yazyev, M. Troyer, D. Vanderbilt, B. A. Bernevig, and A. A. Soluyanov
  Z2Pack: Numerical Implementation of Hybrid Wannier Centers for Identifying Topological Materials
  arXiv:1610.08983, *to be published in* Physical Review B (2017), http://z2pack.ethz.ch.
  Group(s): Troyer, Yazyev / Project(s): VP1

- T. Bzdušek, Q. Wu, A. Rüegg, M. Sigrist, and A. A. Soluyanov
  Nodal-chain metals
  Nature **538**, 75 (2016).
  Group(s): Troyer / Project(s): VP1

- S. M. Griffin, P. Staar, T. C. Schulthess, M. Troyer, and N. A. Spaldin
  A bespoke single-band Hubbard model material
  Physical Review B **93**, 075115 (2016).
  Group(s): Schulthess, Spaldin, Troyer / Project(s): VP1

- A. A. Soluyanov, D. Gresch, M. Troyer, R. M. Lutchyn, B. Bauer, and C. Nayak
  Optimizing spin-orbit splittings in InSb Majorana nanowires
  Physical Review B **93**, 115317 (2016).
  Group(s): Troyer / Project(s): VP1

- F. Y. Bruno, A. Tamai, Q. S. Wu, I. Cucchi, C. Barreteau, A. de la Torre, S. McKeown Walker, S. Riccò, Z. Wang, T. K. Kim, M. Hoesch, M. Shi, N. C. Plumb, E. Giannini, A. A. Soluyanov, and F. Baumberger
  Observation of large topologically trivial Fermi arcs in the candidate type-II Weyl semimetal WTe_2
  Physical Review B **94**, 121112 (2016).
  Group(s): Troyer / Project(s): VP1

  V. E. Sacksteder and Q. Wu
  Quantum interference effects in topological nanowires in a longitudinal magnetic field
  Physical Review B **94**, 205424 (2016).
  Group(s): Troyer / Project(s): VP1

- G. W. Winkler, A. A. Soluyanov, and M. Troyer
  Smooth gauge and Wannier functions for topological band structures in arbitrary dimensions
  Physical Review B **93**, 035453 (2016).
  Group(s): Troyer / Project(s): VP1

- Z. Wang, D. Gresch, A. A. Soluyanov, W. Xie, S. Kushwaha, X. Dai, M. Troyer, R. J. Cava, and B. A. Bernevig
  $MoTe_2$: a type-II Weyl topological metal
  Physical Review Letters **117**, 056805 (2016).
  Group(s): Troyer / Project(s): VP1

- G. W. Winkler, Q. Wu, M. Troyer, P. Krogstrup, and A. A. Soluyanov
  Topological Phases in $InAs_{1-x}Sb_x$: From Novel Topological Semimetal to Majorana Wire
  Physical Review Letters **117**, 076403 (2016).
  Group(s): Troyer / Project(s): VP1

- G. Autès, D. Gresch, M. Troyer, A. A. Soluyanov, and O. V. Yazyev
  Robust Type-II Weyl Semimetal Phase in Transition Metal Diphosphides XP_2 (X = Mo, W)
  Physical Review Letters **117**, 066402 (2016).
  Group(s): Troyer, Yazyev / Project(s): VP1

- Z. Zhu, G. W. Winkler, Q. Wu, J. Li, and A. A. Soluyanov
  Triple Point Topological Metals
  Physical Review X **6**, 031003 (2016).
  Group(s): Troyer / Project(s): VP1

- A. Tamai, Q. S. Wu, I. Cucchi, F. Y. Bruno, S. Riccò, T. K. Kim, M. Hoesch, C. Barreteau, E. Giannini, C. Besnard, A. A. Soluyanov, and F. Baumberger
  Fermi Arcs and Their Topological Character in the Candidate Type-II Weyl Semimetal $MoTe_2$
  Physical Review X **6**, 031021 (2016).
  Group(s): Troyer / Project(s): VP1

- M. Iazzi, A. A. Soluyanov, and M. Troyer
  Topological origin of the fermion sign problem
  Physical Review B **93**, 115102 (2016).
  Group(s): Troyer / Project(s): HP3, VP1

- A. A. Soluyanov, D. Gresch, Z. Wang, Q. Wu, M. Troyer, X. Dai, and B. A. Bernevig
  Type-II Weyl semimetals
  Nature **527**, 495 (2015).
  Group(s): Troyer / Project(s): VP1

- M. Iazzi and M. Troyer
  Efficient continuous-time quantum Monte Carlo algorithm for fermionic lattice models
  Physical Review B **91**, 241118 (2015).
  Group(s): Troyer / Project(s): HP3, VP1

- L. Wang, M. Iazzi, P. Corboz, and M. Troyer
  Efficient continuous-time quantum Monte Carlo method for the ground state of correlated fermions
  Physical Review B **91**, 235151 (2015).
  Group(s): Troyer / Project(s): HP3, VP1

- H. Shinaoka, M. Troyer, and P. Werner
  Accuracy of downfolding based on the constrained random-phase approximation
  Physical Review B **91**, 245156 (2015).
  Group(s): Troyer, Werner / Project(s): VP1, HP3

  Y.-H. Liu and L. Wang
  Quantum Monte Carlo study of mass-imbalanced Hubbard models
  Physical Review B **92**, 235129 (2015).
  Group(s): Troyer / Project(s): HP3, VP1

- H. Shinaoka, Y. Nomura, S. Biermann, M. Troyer, and P. Werner
  Negative sign problem in continuous-time quantum Monte Carlo: optimal choice of single-particle basis for impurity problems
  Physical Review B **92**, 195126 (2015).
  Group(s): Troyer, Werner / Project(s): HP3, VP1

- L. Wang, H. Shinaoka, and M. Troyer
  Fidelity Susceptibility Perspective on the Kondo Effect and Impurity Quantum Phase Transitions
  Physical Review Letters **115**, 236601 (2015).
  Group(s): Troyer / Project(s): HP3, VP1

  L. Wang, Y.-H. Liu, M. Iazzi, M. Troyer, and G. Harcos
  Split Orthogonal Group: A Guiding Principle for Sign-Problem-Free Fermionic Simulations
  Physical Review Letters **115**, 250601 (2015).
  Group(s): Troyer / Project(s): HP3, VP1

- H. Shinaoka, S. Hoshino, M. Troyer, and P. Werner
  Phase Diagram of Pyrochlore Iridates: All-in–All-out Magnetic Ordering and Non-Fermi-Liquid Properties
  Physical Review Letters **115**, 156401 (2015).
  Group(s): Troyer, Werner / Project(s): VP1, HP3

- L. Wang, Y.-H. Liu, J. Imriška, P. N. Ma, and M. Troyer
  Fidelity Susceptibility Made Simple: A Unified Quantum Monte Carlo Approach
  Physical Review X **5**, 031007 (2015).
  Group(s): Troyer / Project(s): HP3, VP1

  S. Keller, M. Dolfi, M. Troyer, and M. Reiher
  An efficient matrix product operator representation of the quantum chemical Hamiltonian
  The Journal of Chemical Physics **143**, 244118 (2015).
  Group(s): Troyer / Project(s): HP3

- L. Wang and M. Troyer
  Renyi Entanglement Entropy of Interacting Fermions Calculated Using the Continuous-Time Quantum Monte Carlo Method
  Physical Review Letters **113**, 110401 (2014).
  Group(s): Troyer / Project(s): VP1, HP3

Group of Dirk van der Marel

- A. Stucky, G. W. Scheerer, Z. Ren, D. Jaccard, J.-M. Poumirol, C. Barreteau, E. Giannini, and D. van der Marel
  Isotope effect in superconducting n-doped $SrTiO_3$
  Scientific Reports **6**, 37582 (2016).
  Group(s): van der Marel / Project(s): PF7

- J. Ruppen, J. Teyssier, O. E. Peil, S. Catalano, M. Gibert, J. Mravlje, J.-M. Triscone, A. Georges, and D. van der Marel
  Optical spectroscopy and the nature of the insulating state of rare-earth nickelates
  Physical Review B **92**, 155145 (2015).
  Group(s): Georges, van der Marel / Project(s): VP1, PP7

Group of Joost VandeVondele

- V. V. Rybkin and J. VandeVondele
  Spin-Unrestricted Second-Order Møller-Plesset (MP2) Forces for the Condensed Phase: From Molecular Radicals to F-Centers in Solids
  Journal of Chemical Theory and Computation **12**, 2214 (2016).
  Group(s): VandeVondele / Project(s): HP3

  D. S. Tikhonov, A. A. Otlyotov, and V. V. Rybkin
  The effect of molecular dynamics sampling on the calculated observable gas-phase structures
  Physical Chemistry Chemical Physics **18**, 18237 (2016).
  Group(s): VandeVondele / Project(s): HP3

  D. S. Tikhonov, D. I. Sharapa, J. Schwabedissen, and V. V. Rybkin
  Application of classical simulations for the computation of vibrational properties of free molecules
  Physical Chemistry Chemical Physics **18**, 28325 (2016).
  Group(s): VandeVondele / Project(s): HP3

- J. Cheng and J. VandeVondele
  Calculation of Electrochemical Energy Levels in Water Using the Random Phase Approximation and a Double Hybrid Functional
  Physical Review Letters **116**, 086402 (2016).
  Group(s): VandeVondele / Project(s): HP3

- V. Kapil, J. VandeVondele, and M. Ceriotti
  Accurate molecular dynamics and nuclear quantum effects at low cost by multiple steps in real and imaginary time: Using density functional theory to accelerate wavefunction methods
  The Journal of Chemical Physics **144**, 054111 (2016).
  Group(s): Ceriotti, VandeVondele / Project(s): HP3,HP4

- M. Del Ben, O. Schütt, T. Wentz, P. Messmer, J. Hutter, and J. VandeVondele
  Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution
  Computer Physics Communications **187**, 120 (2015).
  Group(s): Hutter, VandeVondele / Project(s): HP3

- M. Del Ben, J. Hutter, and J. VandeVondele
  Forces and stress in second order Møller-Plesset perturbation theory for condensed phase systems within the resolution-of-identity Gaussian and plane waves approach
  The Journal of Chemical Physics **143**, 102803 (2015).
  Group(s): Hutter, VandeVondele / Project(s): HP3

- M. Del Ben, J. Hutter, and J. VandeVondele
  Probing the structural and dynamical properties of liquid water with models including non-local electron correlation
  The Journal of Chemical Physics **143**, 054506 (2015).
  Group(s): Hutter, VandeVondele / Project(s): HP3

U. Borštnik, J. VandeVondele, V. Weber, and J. Hutter
Sparse matrix multiplication: The distributed block-compressed sparse row library
Parallel Computing **40**, 47 (2014).
Group(s): Hutter, VandeVondele / Project(s): HP3

Group of Anatole von Lilienfeld

- A. Solovyeva and O. A. von Lilienfeld
  Alchemical Screening of Ionic Crystals
  Physical Chemistry Chemical Physics **18**, 31078 (2016).
  Group(s): von Lilienfeld / Project(s): HP5

- F. A. Faber, A. Lindmaa, O. A. von Lilienfeld, and R. Armiento
  Machine Learning Energies of 2 Million Elpasolite (ABC_2D_6) Crystals
  Physical Review Letters **117**, 135502 (2016).
  Group(s): von Lilienfeld / Project(s): HP5

M. to Baben, J. O. Achenbach, and O. A. von Lilienfeld
Guiding ab initio *calculations by alchemical derivatives*
The Journal of Chemical Physics **144**, 104103 (2016).
Group(s): von Lilienfeld / Project(s): HP5

K. Y. S. Chang, S. Fias, R. Ramakrishnan, and O. A. von Lilienfeld
Fast and accurate predictions of covalent bonds in chemical space
The Journal of Chemical Physics **144**, 174110 (2016).
Group(s): von Lilienfeld / Project(s): HP5

B. Huang and O. A. von Lilienfeld
Understanding molecular representations in machine learning: The role of uniqueness and target similarity
The Journal of Chemical Physics **145**, 161102 (2016).
Group(s): von Lilienfeld / Project(s): HP5

Y. S. Al-Hamdani, D. Alfè, O. A. von Lilienfeld, and A. Michaelides
Tuning dissociation using isoelectronically doped graphene and hexagonal boron nitride: Water and other small molecules
The Journal of Chemical Physics **144**, 154706 (2016).
Group(s): von Lilienfeld / Project(s): HP5

R. Ramakrishnan and O. A. von Lilienfeld
Many Molecular Properties from One Kernel in Chemical Space
CHIMIA **69**, 182 (2015).
Group(s): von Lilienfeld / Project(s): HP5

O. A. von Lilienfeld, R. Ramakrishnan, M. Rupp, and A. Knoll
Fourier series of atomic radial distribution functions: A molecular fingerprint for machine learning models of quantum chemical properties
International Journal of Quantum Chemistry **115**, 1084 (2015).
Group(s): von Lilienfeld / Project(s): HP5

- F. Faber, A. Lindmaa, O. A. von Lilienfeld, and R. Armiento
  Crystal Structure Representations for Machine Learning Models of Formation Energies
  International Journal of Quantum Chemistry **115**, 1094 (2015).
  Group(s): von Lilienfeld / Project(s): HP5

T. Bereau, D. Andrienko, and O. A. von Lilienfeld
Transferable atomic multipole machine learning models for small organic molecules
Journal of Chemical Theory and Computation **11**, 3225 (2015).
Group(s): von Lilienfeld / Project(s): HP5

P. O. Dral, O. A. von Lilienfeld, and W. Thiel
Machine Learning of Parameters for Accurate Semiempirical Quantum Chemical Calculations
Journal of Chemical Theory and Computation **11**, 2120 (2015).
Group(s): von Lilienfeld / Project(s): HP5

R. Ramakrishnan, P. O. Dral, M. Rupp, and O. A. von Lilienfeld
Big Data Meets Quantum Chemistry Approximations: The Δ-Machine Learning Approach
Journal of Chemical Theory and Computation **11**, 2087 (2015).
Group(s): von Lilienfeld / Project(s): HP4

R. Ramakrishnan, M. Hartmann, E. Tapavicza, and O. A. von Lilienfeld
Electronic Spectra from TDDFT and Machine Learning in Chemical Space
The Journal of Chemical Physics **143**, 084111 (2015).
Group(s): von Lilienfeld / Project(s): HP5

M. Rupp, R. Ramakrishnan, and O. A. von Lilienfeld
Machine Learning for Quantum Mechanical Properties of Atoms in Molecules
The Journal of Physical Chemistry Letters **6**, 3309 (2015).
Group(s): von Lilienfeld / Project(s): HP5

K. Hansen, F. Biegler, R. Ramakrishnan, W. Pronobis, O. A. von Lilienfeld, K.-R. Müller, and A. Tkatchenko
Machine Learning Predictions of Molecular Properties: Accurate Many-Body Potentials and Nonlocality in Chemical Space
The Journal of Physical Chemistry Letters **6**, 2326 (2015).
Group(s): von Lilienfeld / Project(s): HP5

R. Ramakrishnan, P. O. Dral, M. Rupp, and O. A. von Lilienfeld
Quantum chemistry structures and properties of 134 kilo molecules
Scientific Data **1**, 140022 (2014).
Group(s): von Lilienfeld / Project(s): HP4

K. Y. S. Chang and O. A. von Lilienfeld
Quantum Mechanical Treatment of Variable Molecular Composition: From 'Alchemical' Changes of State Functions to Rational Compound Design
CHIMIA International Journal for Chemistry **68**, 602 (2014).
Group(s): von Lilienfeld / Project(s): HP4

Group of Philipp Werner

H. Shinaoka, E. Gull, and P. Werner
Continuous-time hybridization expansion quantum impurity solver for multi-orbital systems with complex hybridizations
Computer Physics Communications (2017), doi:10.1016/j.cpc.2017.01.003.
Group(s): Werner / Project(s): HP3

P. Werner and M. Casula
Dynamical screening in correlated electron systems - From lattice models to realistic materials
Journal of Physics: Condensed Matter **28**, 383001 (2016).
Group(s): Werner / Project(s): HP3

P. Werner, S. Hoshino, and H. Shinaoka
Spin-freezing perspective on cuprates
Physical Review B **94**, 245134 (2016).
Group(s): Werner / Project(s): HP3

L. Huang, Y. Wang, L. Wang, and P. Werner
Detecting phase transitions and crossovers in Hubbard models using the fidelity susceptibility
Physical Review B **94**, 235110 (2016).
Group(s): Werner / Project(s): HP3

D. Golež, P. Werner, and M. Eckstein
Photoinduced gap closure in an excitonic insulator
Physical Review B **94**, 035121 (2016).
Group(s): Werner / Project(s): HP3

Y. Murakami, P. Werner, N. Tsuji, and H. Aoki
Damping of the collective amplitude mode in superconductors with strong electron-phonon coupling
Physical Review B **94**, 115126 (2016).
Group(s): Werner / Project(s): HP3

Y. Murakami, P. Werner, N. Tsuji, and H. Aoki
Multiple amplitude modes in strongly coupled phonon-mediated superconductors
Physical Review B **93**, 094509 (2016).
Group(s): Werner / Project(s): HP3

- L. Boehnke, F. Nilsson, F. Aryasetiawan, and P. Werner
  When strong correlations become weak: Consistent merging of GW and DMFT
  Physical Review B **94**, 201106 (2016).
  Group(s): Werner / Project(s): HP3

  D. Golež, M. Eckstein, and P. Werner
  Dynamics of screening in photodoped Mott insulators
  Physical Review B **92**, 195123 (2015).
  Group(s): Werner / Project(s): HP3

  Y. Murakami, P. Werner, N. Tsuji, and H. Aoki
  Interaction quench in the Holstein model: Thermalization crossover from electron- to phonon-dominated relaxation
  Physical Review B **91**, 045128 (2015).
  Group(s): Werner / Project(s): HP3

- H. Shinaoka, M. Troyer, and P. Werner
  Accuracy of downfolding based on the constrained random-phase approximation
  Physical Review B **91**, 245156 (2015).
  Group(s): Troyer, Werner / Project(s): VP1, HP3

- H. Shinaoka, Y. Nomura, S. Biermann, M. Troyer, and P. Werner
  Negative sign problem in continuous-time quantum Monte Carlo: optimal choice of single-particle basis for impurity problems
  Physical Review B **92**, 195126 (2015).
  Group(s): Troyer, Werner / Project(s): HP3, VP1

  P. Werner, R. Sakuma, F. Nilsson, and F. Aryasetiawan
  Dynamical screening in La_2CuO_4
  Physical Review B **91**, 125142 (2015).
  Group(s): Werner / Project(s): HP3

- H. Shinaoka, S. Hoshino, M. Troyer, and P. Werner
  Phase Diagram of Pyrochlore Iridates: All-in–All-out Magnetic Ordering and Non-Fermi-Liquid Properties
  Physical Review Letters **115**, 156401 (2015).
  Group(s): Troyer, Werner / Project(s): VP1, HP3

  L. Huang, T. Ayral, S. Biermann, and P. Werner
  Extended dynamical mean-field study of the Hubbard model with long-range interactions
  Physical Review B **90**, 195114 (2014).
  Group(s): Werner / Project(s): HP3

Group of Oleg Yazyev

- D. Gresch, G. Autès, O. V. Yazyev, M. Troyer, D. Vanderbilt, B. A. Bernevig, and A. A. Soluyanov
  Z2Pack: Numerical Implementation of Hybrid Wannier Centers for Identifying Topological Materials
  arXiv:1610.08983, *to be published in* Physical Review B (2017), http://z2pack.ethz.ch.
  Group(s): Troyer, Yazyev / Project(s): VP1

  G. Manzoni, A. Crepaldi, G. Autès, A. Sterzi, F. Cilento, A. Akrap, I. Vobornik, L. Gragnaniello, P. Bugnon, M. Fonin, H. Berger, M. Zacchigna, O. V. Yazyev, and F. Parmigiani
  Temperature dependent non-monotonic bands shift in $ZrTe_5$
  Journal of Electron Spectroscopy and Related Phenomena (2016), doi:10.1016/j.elspec.2016.09.006.
  Group(s): Yazyev / Project(s): VP1

- N. Xu, H. M. Weng, B. Q. Lv, C. E. Matt, J. Park, F. Bisti, V. N. Strocov, D. Gawryluk, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, G. Autès, O. V. Yazyev, Z. Fang, X. Dai, T. Qian, J. Mesot, H. Ding, and M. Shi
  Observation of Weyl nodes and Fermi arcs in tantalum phosphide
  Nature Communications **7**, 11006 (2016).
  Group(s): Shi, Yazyev / Project(s): PP7, VP1

  B. Náfrádi, P. Szirmai, M. Spina, H. Lee, O. V. Yazyev, A. Arakcheeva, D. Chernyshov, M. Gibert, L. Forró, and E. Horváth
  Optically switched magnetism in photovoltaic perovskite $CH_3NH_3(Mn:Pb)I_3$
  Nature Communications **7**, 13406 (2016).
  Group(s): Yazyev / Project(s): VP1

- G. Autès, A. Isaeva, L. Moreschini, J. C. Johannsen, A. Pisoni, R. Mori, W. Zhang, T. G. Filatova, A. N. Kuznetsov, L. Forró, W. Van den Broek, Y. Kim, K. S. Kim, A. Lanzara, J. D. Denlinger, E. Rotenberg, A. Bostwick, M. Grioni, and O. V. Yazyev
  A novel quasi-one-dimensional topological insulator in bismuth iodide β-Bi_4I_4
  Nature Materials **15**, 154 (2016).
  Group(s): Yazyev / Project(s): VP1

  L. Yang, M. Jeong, A. Arakcheeva, I. Živković, B. Náfrádi, A. Magrez, A. Pisoni, J. Jacimovic, V. M. Katukuri, S. Katrych, N. E. Shaik, O. V. Yazyev,

L. Forró, and H. M. Rønnow
Possibility of an unconventional spin state of Ir^{4+} in $Ba_{21}Ir_9O_{43}$ single crystal
Physical Review B **94**, 104403 (2016).
Group(s): Yazyev / Project(s): VP1

G. Autès, D. Gresch, M. Troyer, A. A. Soluyanov, and O. V. Yazyev
Robust Type-II Weyl Semimetal Phase in Transition Metal Diphosphides XP_2 ($X = Mo, W$)
Physical Review Letters **117**, 066402 (2016).
Group(s): Troyer, Yazyev / Project(s): VP1

G. Manzoni, L. Gragnaniello, G. Autès, T. Kuhn, A. Sterzi, F. Cilento, M. Zacchigna, V. Enenkel, I. Vobornik, L. Barba, F. Bisti, P. Bugnon, A. Magrez, V. N. Strocov, H. Berger, O. V. Yazyev, M. Fonin, F. Parmigiani, and A. Crepaldi
Evidence for a Strong Topological Insulator Phase in $ZrTe_5$
Physical Review Letters **117**, 237601 (2016).
Group(s): Yazyev / Project(s): VP1

P. Babkevich, V. M. Katukuri, B. Fåk, S. Rols, T. Fennell, D. Pajić, H. Tanaka, T. Pardini, R. R. P. Singh, A. Mitrushchenkov, O. V. Yazyev, and H. M. Rønnow
Magnetic excitations and electronic interactions in Sr_2CuTeO_6: A spin-1/2 square lattice Heisenberg antiferromagnet
Physical Review Letters **117**, 237203 (2016).
Group(s): Yazyev / Project(s): VP1

J. C. Johannsen, G. Autès, A. Crepaldi, S. Moser, B. Casarin, F. Cilento, M. Zacchiagna, H. Berger, A. Magrez, P. Bugnon, J. Avila, M. C. Asensio, F. Parmigiani, O. V. Yazyev, and M. Grioni
Engineering the topological surface states in the $(Sb_2)_m$-Sb_2Te_3 ($m = 0 - 3$) superlattice series
Physical Review B **91**, 201101 (2015).
Group(s): Yazyev / Project(s): VP1

2. Scientific articles in journals without peer review

Group of Antoine Georges

D. Sutter, C. G. Fatuzzo, S. Moser, M. Kim, R. Fittipaldi, A. Vecchione, V. Granata, Y. Sassa, F. Cossalter, G. Gatti, M. Grioni, H. M. Rønnow, N. C. Plumb, C. E. Matt, M. Shi, M. Hoesch, T. K. Kim, T.-R. Chang, H.-T. Jeng, C. Jozwiak, A. Bostwick, E. Rotenberg, A. Georges, T. Neupert, and J. Chang
Hallmarks of Hund's coupling in the Mott insulator Ca_2RuO_4
arXiv:1610.02854 (2016).
Group(s): Georges / Project(s): VP1

Group of Jürg Hutter

O. Schütt, P. Messmer, J. Hutter, and J. VandeVondele
GPU-Accelerated Sparse Matrix-Matrix Multiplication for Linear Scaling Density Functional Theory
in *Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics*, R. C. Walker and A. W. Götz, eds. (John Wiley & Sons, Ltd, Chichester, 2016), p. 173.
Group(s): Hutter,VandeVondele / Project(s): HP3

Group of Christoph Koch

- A. Shaikhha, M. Dashti, and C. Koch
Push vs. Pull-Based Loop Fusion in Query Engines
arXiv:1610.09166 (2016).
Group(s): Koch / Project(s): HP5

- A. Shaikhha, Y. Klonatos, and C. Koch
Building Efficient Query Engines in a High-Level Language
arXiv:1612.05566 (2016).
Group(s): Koch / Project(s): HP5

Group of Nicola Marzari

D. Dragoni, D. Ceresoli, and N. Marzari
Vibrational and thermoelastic properties of bcc iron from selected EAM potentials
arXiv:1605.03334 (2016).
Group(s): Marzari / Project(s): VP2

- N. Mounet, M. Gibertini, P. Schwaller, A. Merkys, I. E. Castelli, A. Cepellotti, G. Pizzi, and N. Marzari
Novel two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds
arXiv:1611.05234 (2016).
Group(s): Marzari / Project(s): VP2

Group of Daniele Passerone

- L. Talirz, P. Shinde, D. Passerone, and C. A. Pignedoli
Synthesis of Atomically Precise Graphene-Based Nanostructures: A Simulation Point of View
in *On-Surface Synthesis*, A. Gourdon, ed. (Springer International Publishing, 2016), Advances in Atom and Single Molecule Machines, p. 237, doi:10.1007/978-3-319-26600-8_12.
Group(s): Passerone / Project(s): VP2

Group of Ursula Röthlisberger

- N. J. Browning, R. Ramakrishnan, O. A. von Lilienfeld, and U. Röthlisberger
Genetic optimization of training sets for improved machine learning models of molecular properties
arXiv:1611.07435 (2016).
Group(s): Röthlisberger, von Lilienfeld / Project(s): VP2

Group of Nicola Spaldin

- 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
arXiv:1610.00783 (2016).
Group(s): Spaldin, Troyer / Project(s): VP1

- A. Scaramucci, H. Shinaoka, M. V. Mostovoy, M. Müller, and C. Mudry
Spiral order from orientationally correlated random bonds in classical XY models
arXiv:1610.00784 (2016).
Group(s): Spaldin, Troyer / Project(s): VP1

Group of Matthias Troyer

- 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

arXiv:1610.00783 (2016).
Group(s): Spaldin, Troyer / Project(s): VP1

- A. Scaramucci, H. Shinaoka, M. V. Mostovoy, M. Müller, and C. Mudry
  Spiral order from orientationally correlated random bonds in classical XY models
  arXiv:1610.00784 (2016).
  Group(s): Spaldin, Troyer / Project(s): VP1

L. Tiemann, S. Mueller, Q. Wu, T. Tschirky, K. Ensslin, W. Wegscheider, M. Troyer, A. A. Soluyanov, and T. Ihn
On the impact of strain on the electronic properties of InAs/GaSb quantum well systems
arXiv:1610.06776 (2016).
Group(s): Troyer / Project(s): VP1

- D. Gresch, Q. Wu, G. W. Winkler, and A. A. Soluyanov
  Hidden Weyl Points in Centrosymmetric Paramagnetic Metals
  arXiv:1611.01858 (2016).
  Group(s): Troyer / Project(s): VP1

Group of Joost VandeVondele

O. Schütt, P. Messmer, J. Hutter, and J. VandeVondele
GPU-Accelerated Sparse Matrix-Matrix Multiplication for Linear Scaling Density Functional Theory
in *Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics*, R. C. Walker and A. W. Götz, eds. (John Wiley & Sons, Ltd, Chichester, 2016), p. 173.
Group(s): Hutter,VandeVondele / Project(s): HP3

Group of Anatole von Lilienfeld

- N. J. Browning, R. Ramakrishnan, O. A. von Lilienfeld, and U. Röthlisberger
  Genetic optimization of training sets for improved machine learning models of molecular properties
  arXiv:1611.07435 (2016).
  Group(s): Röthlisberger, von Lilienfeld / Project(s): VP2

Group of Philipp Werner

L. Huang, Y. Wang, and P. Werner
Orbital-Selective Mott Transition and Evolution of the Zhang-Rice State in Cubic Phase UO_2 Under Pressure
arXiv:1506.06548 (2015).
Group(s): Werner / Project(s): HP3

S. Hoshino and P. Werner
Spontaneous orbital-selective Mott transitions and the Jahn-Teller metal of A_3C_{60}
arXiv:1609.00136 (2016).
Group(s): Werner / Project(s): HP3

3. Publications involving several groups

Publications with peer review

- F. Evangelisti, M. Stiefel, O. Guseva, R. P. Nia, R. Hauert, E. Hack, L. P. H. Jeurgens, F. Ambrosio, A. Pasquarello, P. Schmutz, and C. Cancellieri
  Electronic and structural characterization of barrier-type amorphous aluminium oxide
  Electrochimica Acta **224**, 503 (2017).
  Group(s): Cancellieri, Pasquarello / Project(s): VP2, PP7

M. Taddei, D. Tiana, N. Casati, J. A. van Bokhoven, B. Smit, and M. Ranocchiari
Mixed-linker UiO-66: structure-property relationships revealed by a combination of high-resolution powder X-ray diffraction and density functional theory calculations
Physical Chemistry Chemical Physics **19**, 1551 (2017).
Group(s): Ranocchiari, Smit / Project(s): VP2

- W. Si, D. Pergolesi, F. Haydous, A. Fluri, A. Wokaun, and T. Lippert
  Investigating the behavior of various cocatalysts on $LaTaON_2$ photoanode for visible light water splitting
  Physical Chemistry Chemical Physics **19**, 656 (2017).
  Group(s): Lippert, Pergolesi / Project(s): PP7

- D. Gresch, G. Autès, O. V. Yazyev, M. Troyer, D. Vanderbilt, B. A. Bernevig, and A. A. Soluyanov
  Z2Pack: Numerical Implementation of Hybrid Wannier Centers for Identifying Topological Materials
  arXiv:1610.08983, *to be published in* Physical Review B (2017), http://z2pack.ethz.ch.
  Group(s): Troyer, Yazyev / Project(s): VP1

- S. M. Griffin, P. Staar, T. C. Schulthess, M. Troyer, and N. A. Spaldin
  A bespoke single-band Hubbard model material
  Physical Review B **93**, 075115 (2016).
  Group(s): Schulthess, Spaldin, Troyer / Project(s): VP1

- G. Fisicaro, L. Genovese, O. Andreussi, N. Marzari, and S. Goedecker
  A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments
  The Journal of Chemical Physics **144**, 014103 (2016).
  Group(s): Goedecker, Marzari / Project(s): HP3

- V. Kapil, J. VandeVondele, and M. Ceriotti
  Accurate molecular dynamics and nuclear quantum effects at low cost by multiple steps in real and imaginary time: Using density functional theory to accelerate wavefunction methods
  The Journal of Chemical Physics **144**, 054111 (2016).
  Group(s): Ceriotti, VandeVondele / Project(s): HP3,HP4

R. Petraglia, A. Nicolaï, M. D. Wodrich, M. Ceriotti, and C. Corminboeuf
Beyond Static Structures: Putting Forth REMD as a Tool to Solve Problems in Computational Organic Chemistry
Journal of Computational Chemistry **37**, 83 (2016).
Group(s): Ceriotti, Corminboeuf / Project(s): HP4

G. W. Mann, K. Lee, M. Cococcioni, B. Smit, and J. B. Neaton
First-principles Hubbard U approach for small molecule binding in metal-organic frameworks
The Journal of Chemical Physics **144**, 174104 (2016).
Group(s): Marzari, Smit / Project(s): HP4

P. Staar, M. Jiang, U. R. Hähner, T. C. Schulthess, and T. A. Maier
Interlaced coarse-graining for the dynamic cluster approximation
Physical Review B **93**, 165144 (2016).
Group(s): Curioni, Schulthess / Project(s): HP5

- G. Miceli, J. Hutter, and A. Pasquarello
  Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets
  Journal of Chemical Theory and Computation **12**, 3456 (2016).
  Group(s): Hutter, Pasquarello / Project(s): VP2,HP3

- N. Xu, H. M. Weng, B. Q. Lv, C. E. Matt, J. Park, F. Bisti, V. N. Strocov, D. Gawryluk, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, G. Autès, O. V. Yazyev, Z. Fang, X. Dai, T. Qian, J. Mesot, H. Ding, and M. Shi
  Observation of Weyl nodes and Fermi arcs in tantalum phosphide
  Nature Communications **7**, 11006 (2016).
  Group(s): Shi, Yazyev / Project(s): PP7, VP1

- K. Lejaeghere, G. Bihlmayer, T. Björkman, P. Blaha, S. Blügel, V. Blum, D. Caliste, I. E. Castelli, S. J. Clark, A. Dal Corso, S. de Gironcoli, T. Deutsch, J. K. Dewhurst,

I. Di Marco, C. Draxl, M. Dulak, O. Eriksson, J. A. Flores-Livas, K. F. Garrity, L. Genovese, P. Giannozzi, M. Giantomassi, S. Goedecker, X. Gonze, O. Grånäs, E. K. U. Gross, A. Gulans, F. Gygi, D. R. Hamann, P. J. Hasnip, N. A. W. Holzwarth, D. Iuşan, D. B. Jochym, F. Jollet, D. Jones, G. Kresse, K. Koepernik, E. Küçükbenli, Y. O. Kvashnin, I. L. M. Locht, S. Lubeck, M. Marsman, N. Marzari, U. Nitzsche, L. Nordström, T. Ozaki, L. Paulatto, C. J. Pickard, W. Poelmans, M. I. J. Probert, K. Refson, M. Richter, G.-M. Rignanese, S. Saha, M. Scheffler, M. Schlipf, K. Schwarz, S. Sharma, F. Tavazza, P. Thunström, A. Tkatchenko, M. Torrent, D. Vanderbilt, M. J. van Setten, V. Van Speybroeck, J. M. Wills, J. R. Yates, G.-X. Zhang, and S. Cottenier

Reproducibility in density functional theory calculations of solids

Science **351**, 6280 (2016).

Group(s): Goedecker, Marzari / Project(s): PP6, VP2

- G. Autès, D. Gresch, M. Troyer, A. A. Soluyanov, and O. V. Yazyev

  Robust Type-II Weyl Semimetal Phase in Transition Metal Diphosphides XP_2 (X = Mo, W)

  Physical Review Letters **117**, 066402 (2016).

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

- D. Carlson, Y.-P. Hsieh, E. Collins, L. Carin, and V. Cevher

  Stochastic Spectral Descent for Discrete Graphical Models

  IEEE Journal of Selected Topics in Signal Processing (2016), doi:10.1109/JSTSP.2015.2505684.

  Group(s): Cevher, Koch / Project(s): HP5

- H. Shinaoka, M. Troyer, and P. Werner

  Accuracy of downfolding based on the constrained random-phase approximation

  Physical Review B **91**, 245156 (2015).

  Group(s): Troyer, Werner / Project(s): VP1, HP3

- M. Del Ben, O. Schütt, T. Wentz, P. Messmer, J. Hutter, and J. VandeVondele

  Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution

  Computer Physics Communications **187**, 120 (2015).

  Group(s): Hutter, VandeVondele / Project(s): HP3

- M. Del Ben, J. Hutter, and J. VandeVondele

  Forces and stress in second order Møller-Plesset perturbation theory for condensed phase systems within the resolution-of-identity Gaussian and plane waves approach

  The Journal of Chemical Physics **143**, 102803 (2015).

  Group(s): Hutter, VandeVondele / Project(s): HP3

- M. Morin, A. Scaramucci, M. Bartkowiak, E. Pomjakushina, G. Deng, D. Sheptyakov, L. Keller, J. Rodriguez-Carvajal, N. A. Spaldin, M. Kenzelmann, K. Conder, and M. Medarde

  Incommensurate magnetic structure, Fe/Cu chemical disorder, and magnetic interactions in the high-temperature multiferroic $YBaCuFeO_5$

  Physical Review B **91**, 064408 (2015).

  Group(s): Kenzelmann, Medarde, Spaldin / Project(s): VP1, PP7

- H. Shinaoka, Y. Nomura, S. Biermann, M. Troyer, and P. Werner

  Negative sign problem in continuous-time quantum Monte Carlo: optimal choice of single-particle basis for impurity problems

  Physical Review B **92**, 195126 (2015).

  Group(s): Troyer, Werner / Project(s): HP3, VP1

- J. Ruppen, J. Teyssier, O. E. Peil, S. Catalano, M. Gibert, J. Mravlje, J.-M. Triscone, A. Georges, and D. van der Marel

  Optical spectroscopy and the nature of the insulating state of rare-earth nickelates

  Physical Review B **92**, 155145 (2015).

  Group(s): Georges, van der Marel / Project(s): VP1, PP7

- X. Cheng, E. Fabbri, M. Nachtegaal, I. E. Castelli, M. El Kazzi, R. Haumont, N. Marzari, and T. J. Schmidt

  Oxygen Evolution Reaction on $La_{1-x}Sr_xCoO_3$ Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties

  Chemistry of Materials **27**, 7662 (2015).

  Group(s): Marzari, Schmidt / Project(s): PP7, VP2

- H. Shinaoka, S. Hoshino, M. Troyer, and P. Werner

  Phase Diagram of Pyrochlore Iridates: All-in–All-out Magnetic Ordering and Non-Fermi-Liquid Properties

  Physical Review Letters **115**, 156401 (2015).

  Group(s): Troyer, Werner / Project(s): VP1, HP3

- M. Del Ben, J. Hutter, and J. VandeVondele

Probing the structural and dynamical properties of liquid water with models including non-local electron correlation

The Journal of Chemical Physics **143**, 054506 (2015).

Group(s): Hutter, VandeVondele / Project(s): HP3

A. Ardevol, G. A. Tribello, M. Ceriotti, and M. Parrinello

Probing the Unfolded Configurations of a β-Hairpin Using Sketch-Map

Journal of Chemical Theory and Computation **11**, 1086 (2015).

Group(s): Ceriotti, Parrinello / Project(s): HP4

U. Borštnik, J. VandeVondele, V. Weber, and J. Hutter

Sparse matrix multiplication: The distributed block-compressed sparse row library

Parallel Computing **40**, 47 (2014).

Group(s): Hutter, VandeVondele / Project(s): HP3

Publications without peer review

- N. J. Browning, R. Ramakrishnan, O. A. von Lilienfeld, and U. Röthlisberger

  Genetic optimization of training sets for improved machine learning models of molecular properties

  arXiv:1611.07435 (2016).

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

- 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

  arXiv:1610.00783 (2016).

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

- A. Scaramucci, H. Shinaoka, M. V. Mostovoy, M. Müller, and C. Mudry

  Spiral order from orientationally correlated random bonds in classical XY models

  arXiv:1610.00784 (2016).

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

- D. E. Carlson, E. Collins, Y.-P. Hsieh, L. Carin, and V. Cevher

  Preconditioned Spectral Descent for Deep Learning

  in *Advances in Neural Information Processing Systems 28 (NIPS 2015)*, C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, eds. (2015).

  Group(s): Cevher, Koch / Project(s): HP5

O. Schütt, P. Messmer, J. Hutter, and J. VandeVondele

GPU-Accelerated Sparse Matrix-Matrix Multiplication for Linear Scaling Density Functional Theory

in *Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics*, R. C. Walker and A. W. Götz, eds. (John Wiley & Sons, Ltd, Chichester, 2016), p. 173.

Group(s): Hutter, VandeVondele / Project(s): HP3

Submitted publications

- M. Pichler, J. Szlachetko, I. E. Castelli, N. Marzari, M. Döbeli, A. Wokaun, D. Pergolesi, and T. Lippert

  Determination of conduction and valence band electronic structure of $LaTiO_xN_y$ thin film

  submitted (2016).

  Group(s): Lippert, Marzari, Pergolesi / Project(s): PP7, VP2

D. Lebedev, M. Povia, K. Waltar, P. M. Abdala, I. E. Castelli, E. Fabbri, M. V. Blanco, A. Fedorov, C. Copéret, N. Marzari, and T. Schmidt

Highly Active and Stable Iridium Pyrochlores for Oxygen Evolution Reaction

submitted (2017).

Group(s): Marzari, Schmidt / Project(s): VP2, PP7

M. Pichler, W. Si, F. Haydous, H. Téllez, J. Druce, E. Fabbri, M. El Kazzi, M. Döbeli, A. Wokaun, D. Pergolesi, and T. Lippert

$LaTiO_xN_y$ thin film model systems for photocatalytic water splitting: physicochemical evolution of the solid-liquid interface and the role of the crystallographic orientation

submitted (2016).

Group(s): PP7 / Project(s): Lippert, Pergolesi, Schmidt

A. Fluri, A. Marcolongo, V. Roddatis, A. Wokaun, Daniele Pergolesi, N. Marzari, and T. Lippert

Enhanced Proton Conductivity in Y-doped $BaZrO_3$ via Strain Engineering

submitted (2016).

Group(s): Lippert, Marzari, Pergolesi / Project(s): PP7, VP2

- E. Gilardi, E. Fabbri, L. Bi, J. L. M. Rupp, A. Wokaun, T. Lippert, D. Pergolesi, and E. Traversa

  Effect of dopant — host ionic radii mismatch on acceptor doped barium zirconate microstructure and proton conductivity

submitted (2016).
Group(s): Lippert, Pergolesi, Schmidt / Project(s): PP7

- G. Fisicaro, L. Genovese, O. Andreussi, S. Mandal, N. N. Nair, N. Marzari, and S. Goedecker
  Soft-sphere continuum solvation in electronic-structure calculations
  submitted (2016).
  Group(s): Goedecker, Marzari / Project(s): HP4

N. Xu, G. Autès, C. E. Matt, B. Q. Lv, M. Y. Yao, F. Bisti, V. N. Strocov, D. Gawryluk, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, T. Qian, O. V. Yazyev, J. Mesot, H. Ding, and M. Shi
Distinct evolutions of Weyl fermion quasiparticles and Fermi arcs with bulk band topology in Weyl semimetals
submitted (2016).
Group(s): Shi, Yazyev / Project(s): PP7, VP1

J. Ruppen, J. Teyssier, I. Ardizzone, O. E. Peil, S. Catalano, M. Gibert, J.-M. Triscone, A. Georges, and D. van der Marel
Impact of antiferromagnetism on the optical properties of rare earth nickelates
submitted (2017).
Group(s): Georges, van der Marel / Project(s): PP7, VP1

F. Franco de Carvalho, C. Pignedoli, and I. Tavernelli
TDDFT-Based Spin-Orbit Couplings of 0D, 1D, and 2D Carbon Nanostructures: Static and Dynamical Effects
submitted (2016).
Group(s): Curioni, Passerone / Project(s): VP2

Cover picture

Nodal chain and nodal net of IrF_4 (from T. Bzdušek, Q. Wu, A. Rüegg, M. Sigrist, and A. A. Soluyanov, *Nodal-chain metals*, Nature **538**, 75 (2016), Vertical Project 1).

Acknowledgements

We would like to thank MaNEP, Material with Novel Electronic properties, an NCCR of the first series, and in particular Christophe Berthod at UniGE, for the MaNEP LaTeX style that served as a base to the present MARVEL style.